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                "COGAN DEREK A"/AU OR "COGAN DEREK ALAN"/AU)
L8           78 SEA ABB=ON  PLU=ON  "HAO M"/AU OR "HAO M H"/AU OR "HAO
                MING"/AU OR "HAO MING HONG"/AU
L9           17 SEA ABB=ON  PLU=ON  "QIAN K"/AU OR "QIAN K C"/AU OR ("QIAN
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L12          15 SEA ABB=ON  PLU=ON  L8 AND INHIBIT?
L13           8 SEA ABB=ON  PLU=ON  (L11 OR L12) NOT (L6 OR L10)
                D STAT QUE NOS
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     FILE HCAPLUS

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     FILE COVERS 1907 - 17 Jan 2006  VOL 144 ISS 4
     FILE LAST UPDATED: 16 Jan 2006  (20060116/ED)

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FILE COVERS 1907 - 17 Jan 2006  VOL 144 ISS 4
FILE LAST UPDATED: 16 Jan 2006  (20060116/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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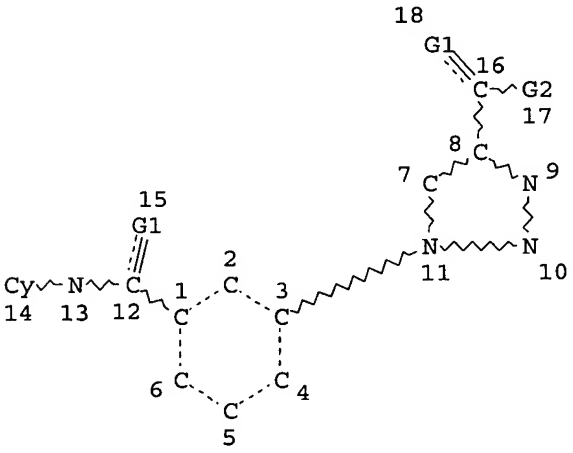


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L6 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:540571 HCAPLUS
DOCUMENT NUMBER: 143:78188
TITLE: Preparation of 1,2,3-triazole amide derivatives as inhibitors of cytokine production
INVENTOR(S): Cogan, Derek; Goldberg, Daniel R.; Hammach, Abdelhakim; Netherton, Matthew Russell; Aungst, Ronald A., Jr.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005056535	A1	20050623	WO 2004-US40306	20041201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005153972	A1	20050714	US 2004-2022	20041201
PRIORITY APPLN. INFO.:			US 2003-526569P P	20031203

OTHER SOURCE(S): MARPAT 143:78188
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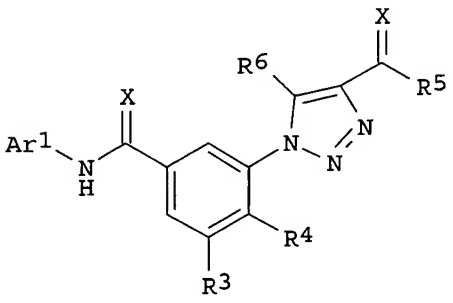


I

AB Title compds. I [Ar1 = heteroaryl, substituted Ph, etc.; R3-6 = H, halo, alkyl, alkoxy, etc.; X = O, S] are prepared For instance,

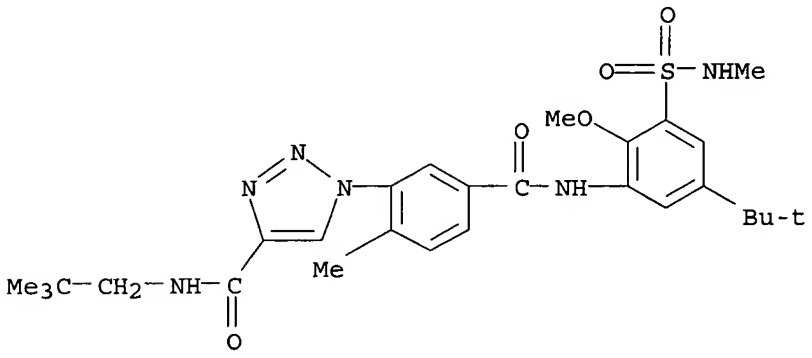
1-[5-[(5-tert-Butyl-2-methoxy-3-methylsulfamoylphenyl)carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide is prepared in 4 steps from 3-azido-4-methylbenzoic acid, Et propiolate and neopentylamine. I inhibit production of cytokines and are thus useful for treating cytokine mediated diseases [no data].

IT **855304-93-7P**, 1-[5-[(5-tert-Butyl-2-methoxy-3-methylsulfamoylphenyl)carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855304-98-2P**, 1-[5-[[5-tert-Butyl-3-(1,3-dioxolan-2-yl)-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-00-9P**, 1-[5-[(5-tert-Butyl-3-formyl-2-methoxyphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-02-1P**, 1-[5-[(5-tert-Butyl-3-dimethylaminomethyl-2-methoxyphenyl)carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-04-3P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-[(4-methylpiperazin-1-yl)methyl]phenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-06-5P**, (S)-1-[5-[[5-tert-Butyl-3-[(3-dimethylaminopyrrolidin-1-yl)methyl]-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-08-7P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-[(morpholin-4-yl)methyl]phenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-10-1P**, 1-[5-[[5-tert-Butyl-3-[[2-(dimethylamino)ethyl]carbamoyl]-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-12-3P**, 1-[5-[[5-tert-Butyl-3-[[(2-dimethylaminoethyl)methylamino]methyl]-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (1-phenylethyl)amide **855305-24-7P**, 1-[5-[[5-tert-Butyl-2-(methanesulfinyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-26-9P**, 1-[5-[(2-tert-Butyl-5-methoxypyridin-4-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-28-1P**, 1-[5-[[5-tert-Butyl-3-[[(2-dimethylaminoethyl)methylamino]methyl]-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-30-5P**, (R)-1-[5-[[5-tert-Butyl-3-[[(2-dimethylaminoethyl)methylamino]methyl]-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid (1-phenylethyl)amide **855305-32-7P**, 1-[5-[(5-tert-Butyl-3-cyano-2-methoxyphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-34-9P**, 1-[5-[[5-tert-Butyl-3-cyano-2-(methanesulfinyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-36-1P**, 1-[5-[(6-tert-Butyl-2-cyano-3-methoxypyridin-4-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-38-3P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-(trifluoromethanesulfonyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-40-7P**, 1-[5-[[5-tert-Butyl-3-(methanesulfinyl)-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-42-9P**, 1-[5-[(5-tert-Butyl-2-methylpyridin-3-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-44-1P**, 1-[5-[[2-tert-Butyl-5-(methanesulfinyl)pyridin-4-yl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-46-3P**, 1-[5-[(6-tert-Butyl-3-oxo-3,4-dihydro-2H-benzo[1,4]oxazin-8-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-

carboxylic acid (2,2-dimethylpropyl)amide **855305-48-5P**, 1-[5-[(5-tert-Butyl-2-methylbenzoxazol-7-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-50-9P**, 1-[5-[(6-tert-Butyl-3,4-dihydro-2H-benzo[1,4]oxazin-8-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-52-1P**, 1-[5-[(5-tert-Butyl-2-oxo-2,3-dihydrobenzoxazol-7-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-54-3P**, 1-[5-[(5-tert-Butyl-2,2-dimethyl-3-oxo-2,3-dihydrobenzofuran-7-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-56-5P**, 1-[5-[[5-tert-Butyl-2-(methylsulfanyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-58-7P**, 1-[5-[[5-tert-Butyl-2-(methanesulfonyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-60-1P**, 1-[5-[(5-tert-Butyl-2-oxo-1,2-dihydropyridin-3-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-62-3P**, 1-[5-[(5-tert-Butyl-1-methyl-2-oxo-1,2-dihydropyridin-3-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-64-5P**, 1-[5-[[5-tert-Butyl-1-[2-(morpholin-4-yl)ethyl]-2-oxo-1,2-dihydropyridin-3-yl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-66-7P**, 1-[5-[(5-tert-Butyl-2-methoxypyridin-3-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-68-9P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-([1,2,3]triazol-1-yl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-70-3P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-(pyrazol-1-yl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-72-5P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-([1,2,4]triazol-1-yl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-74-7P**, 1-[5-[[5-tert-Butyl-3-(imidazol-1-yl)-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-76-9P**, 1-[5-[(5-tert-Butyl-2,3-dimethoxyphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-78-1P**, Methylcarbamic acid 5-tert-butyl-3-[3-[4-(2,2-dimethylpropylcarbamoyl)-[1,2,3]triazol-1-yl]-4-methylbenzoylamino]-2-methoxyphenyl ester **855305-80-5P**, 1-[5-[(5-tert-Butyl-2-methoxy-3-methylphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-82-7P**, 1-[5-[(1-Acetyl-6-methoxy-3,3-dimethyl-2,3-dihydro-1H-indol-5-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-84-9P**, 1-[5-[[5-tert-Butyl-3-(2-carbamoylethyl)-2-methoxyphenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-86-1P**, 1-[5-[[5-tert-Butyl-2-methoxy-3-[2-(morpholin-4-yl)ethyl]phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855305-88-3P**, 1-[5-[(5-tert-Butyl-3-carbamoyl-2-methoxyphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid (2,2-dimethylpropyl)amide **855313-00-7P 855313-01-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,2,3-triazole amide derivs. as inhibitors of cytokine production)

RN 855304-93-7 HCAPLUS

CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylamino)sulfonyl]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



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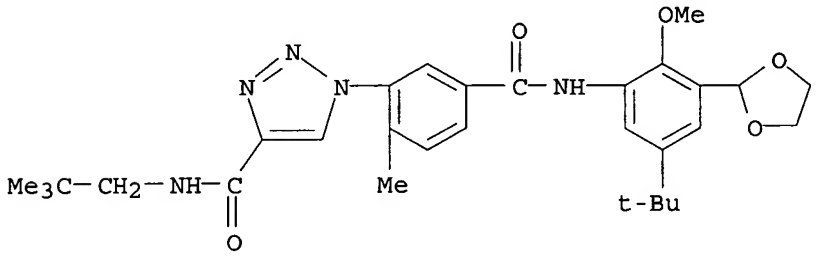

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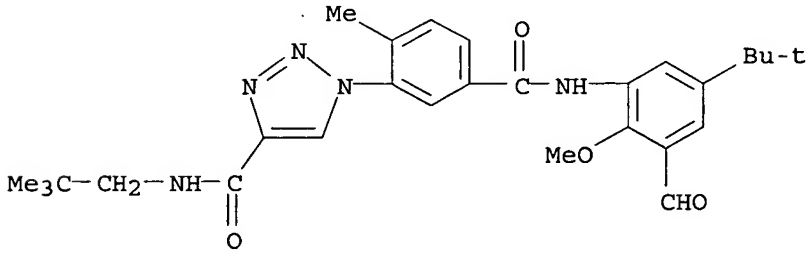

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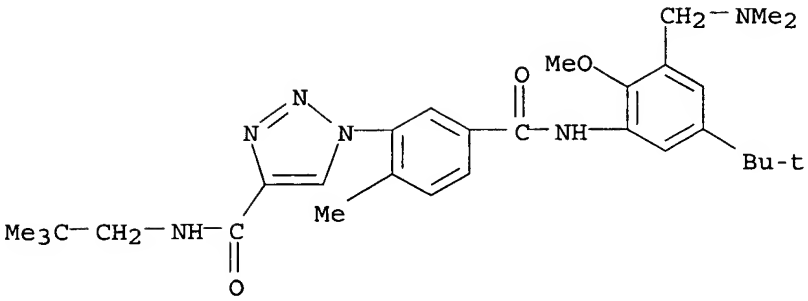

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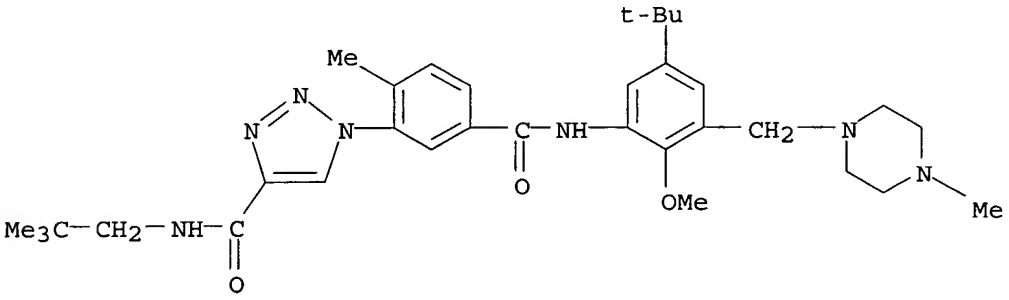

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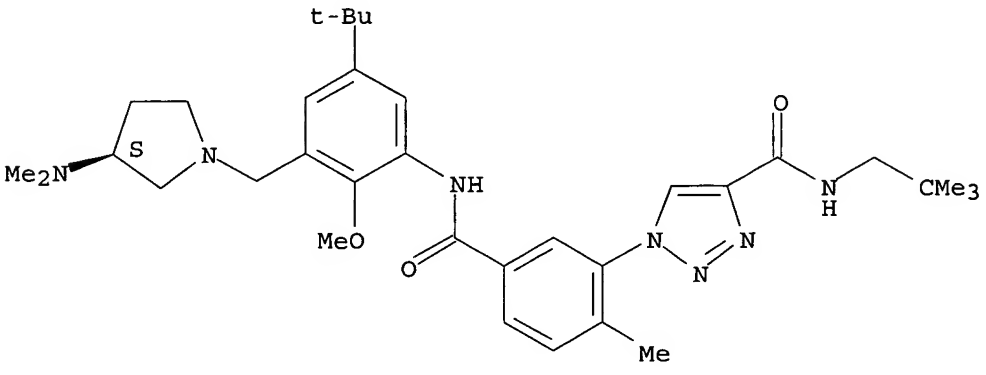
Absolute stereochemistry.



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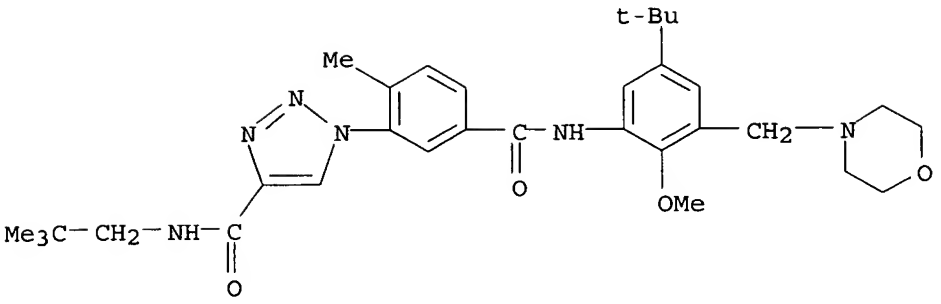

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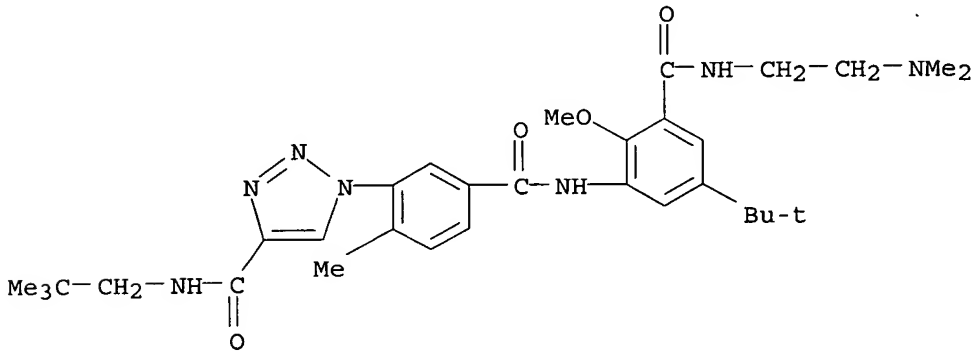

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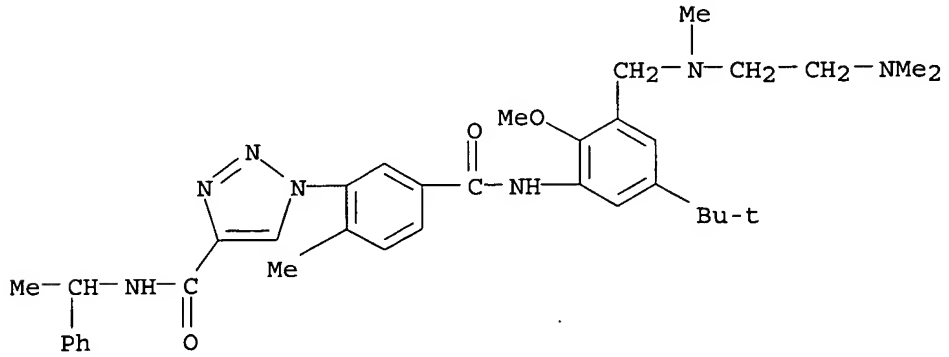

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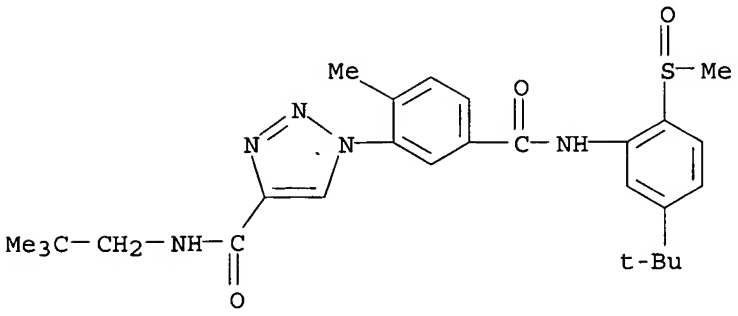
dimethylpropyl)- (9CI) (CA INDEX NAME)



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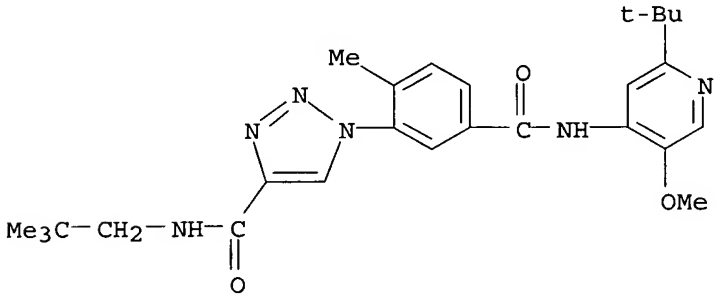

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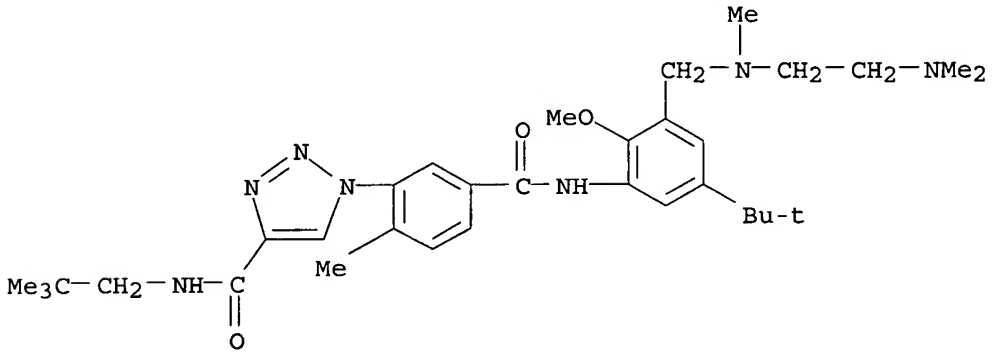
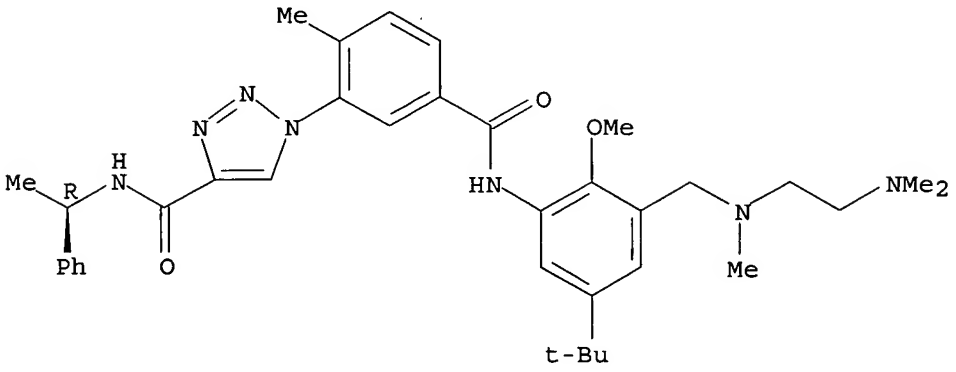


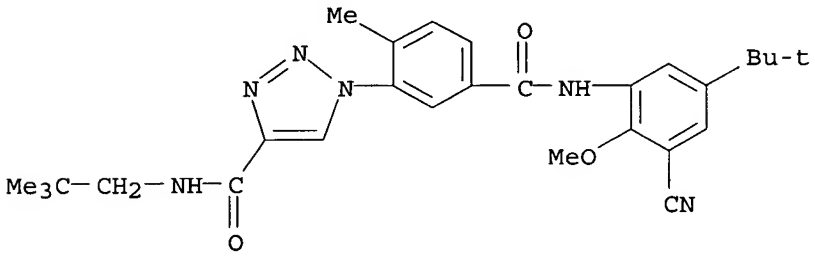
RN 855305-30-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-[[[2-(dimethylamino)ethyl]methylamino]methyl]-5-(1,1-dimethylethyl)-2-

methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1-phenylethyl]-
(9CI) (CA INDEX NAME)

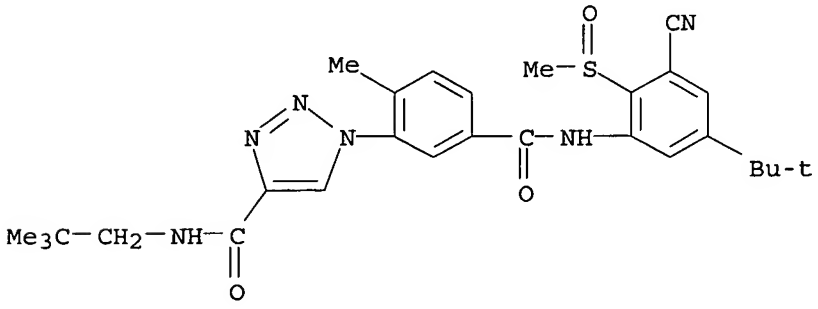
Absolute stereochemistry.



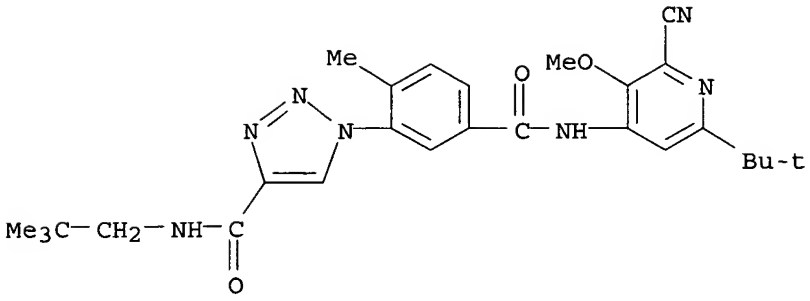
RN 855305-32-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-cyano-5-(1,1-dimethylethyl)-2-
methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)-
(9CI) (CA INDEX NAME)



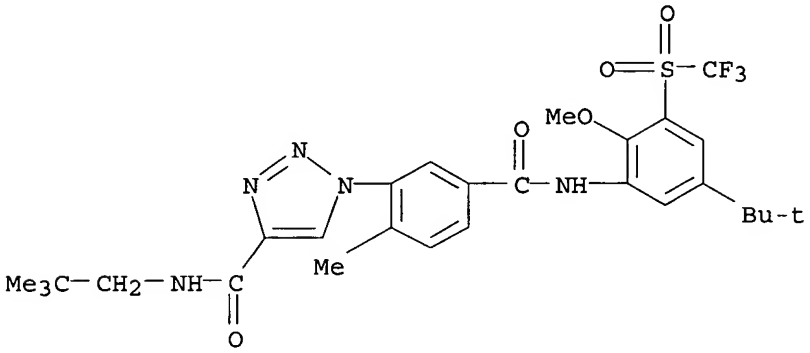
RN 855305-34-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-cyano-5-(1,1-dimethylethyl)-2-
(methylsulfinyl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-
dimethylpropyl)- (9CI) (CA INDEX NAME)



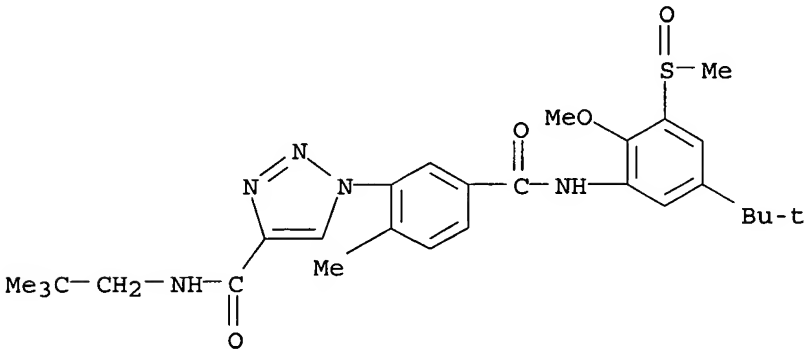
RN 855305-36-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[2-cyano-6-(1,1-dimethylethyl)-3-
methoxy-4-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)-
(9CI) (CA INDEX NAME)



RN 855305-38-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(trifluoromethyl)sulfonyl]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

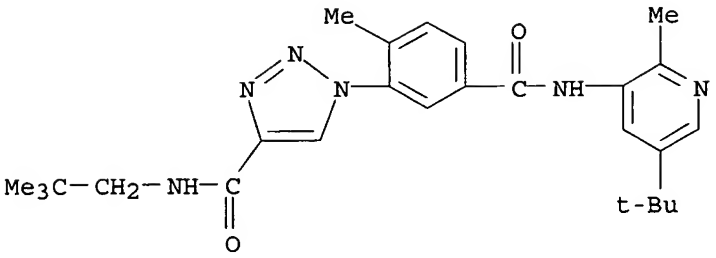


RN 855305-40-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-(methylsulfinyl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

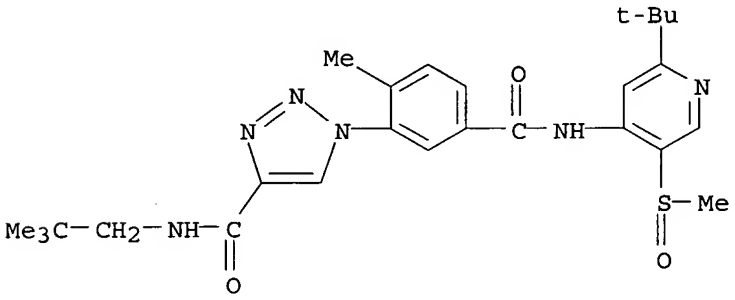


RN 855305-42-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methyl-3-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI)

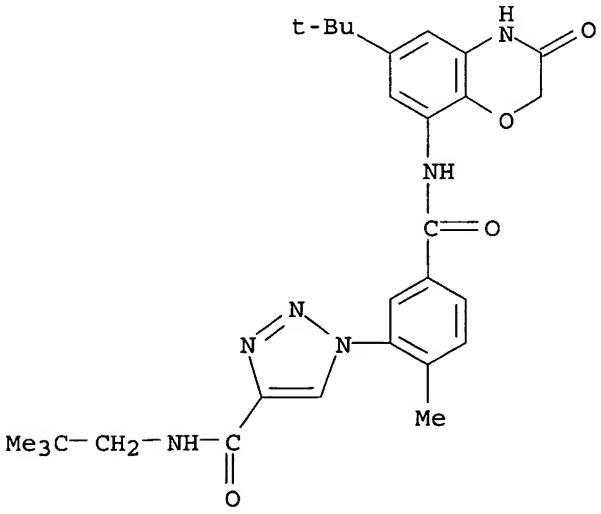
(CA INDEX NAME)



RN 855305-44-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[2-(1,1-dimethylethyl)-5-(methylsulfinyl)-4-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

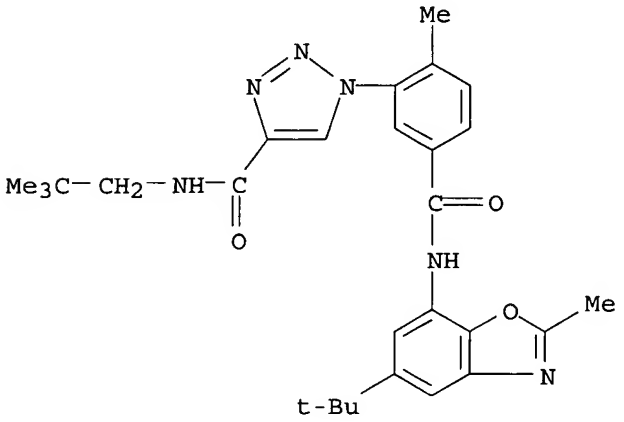


RN 855305-46-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[6-(1,1-dimethylethyl)-3,4-dihydro-3-oxo-2H-1,4-benzoxazin-8-yl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

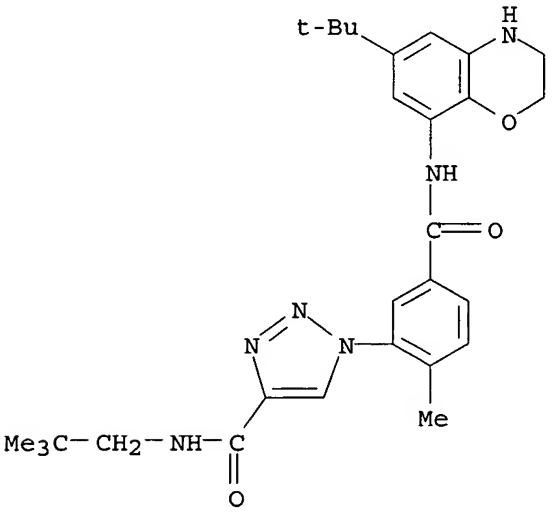


RN 855305-48-5 HCAPLUS

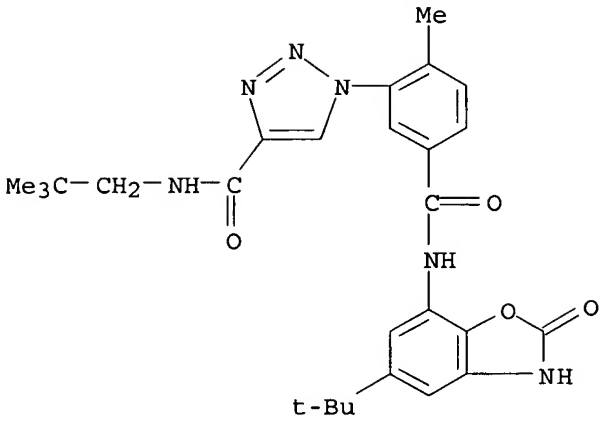
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methyl-7-benzoxazolyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



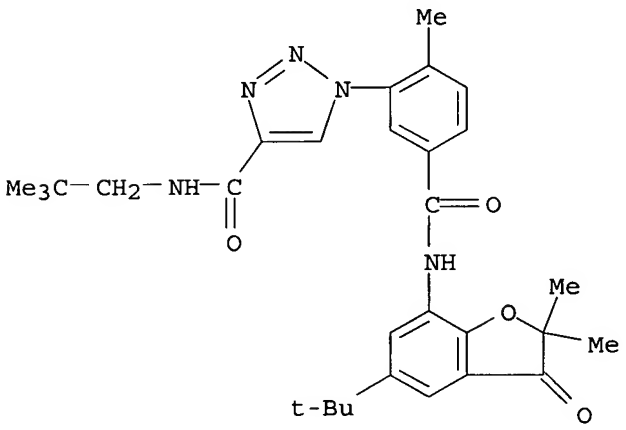
RN 855305-50-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[6-(1,1-dimethylethyl)-3,4-dihydro-2H-1,4-benzoxazin-8-yl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



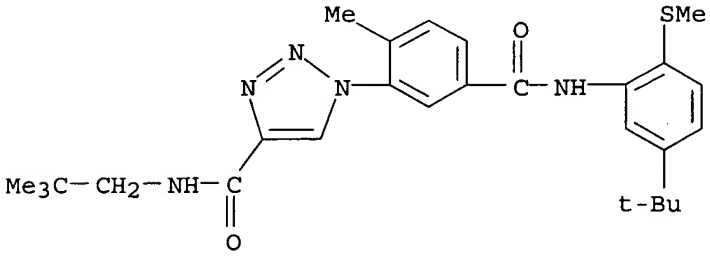
RN 855305-52-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2,3-dihydro-2-oxo-7-benzoxazolyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



RN 855305-54-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2,3-dihydro-2,2-dimethyl-3-oxo-7-benzofuranyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

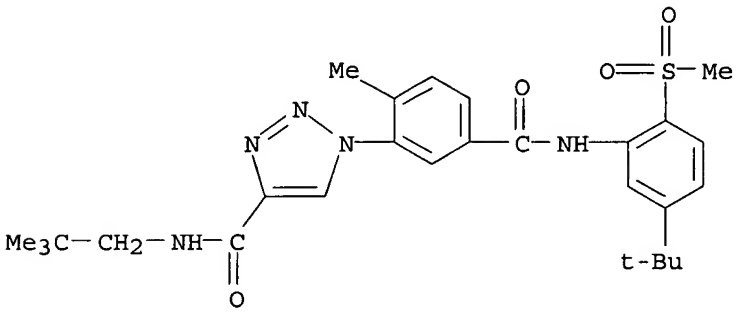


RN 855305-56-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-(methylthio)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

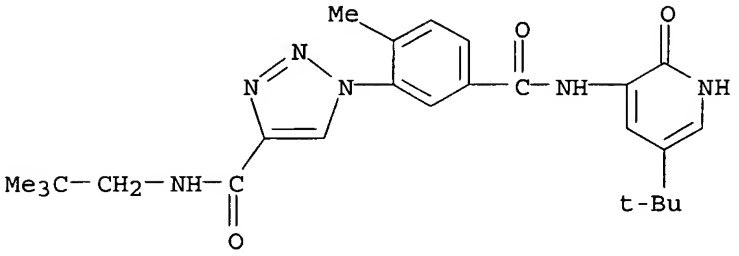


RN 855305-58-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-

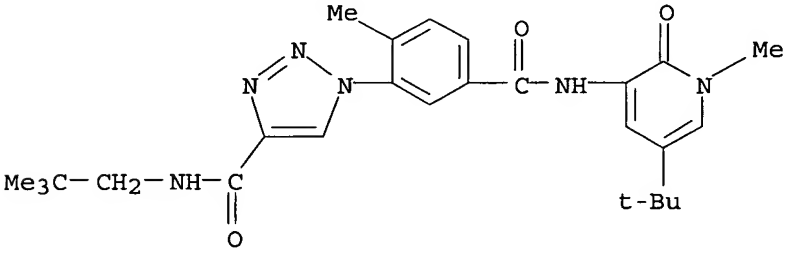
(methylsulfonyl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



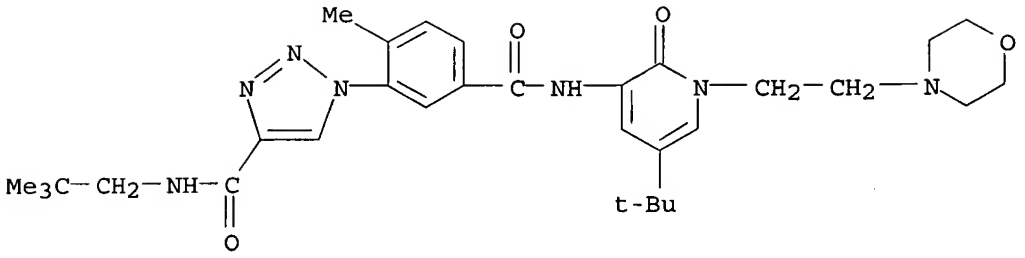
RN 855305-60-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-1,2-dihydro-2-oxo-3-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



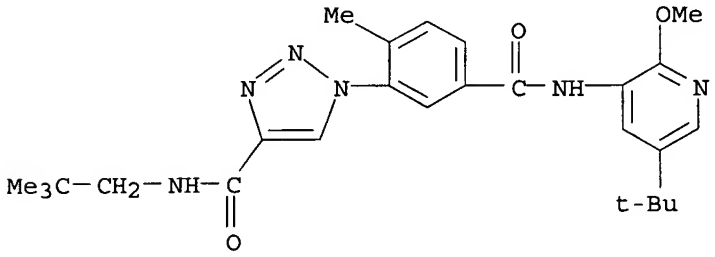
RN 855305-62-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-1,2-dihydro-1-methyl-2-oxo-3-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



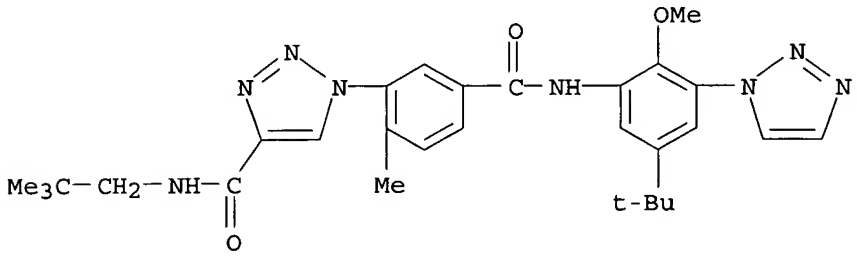
RN 855305-64-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-1,2-dihydro-1-[2-(4-morpholinyl)ethyl]-2-oxo-3-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



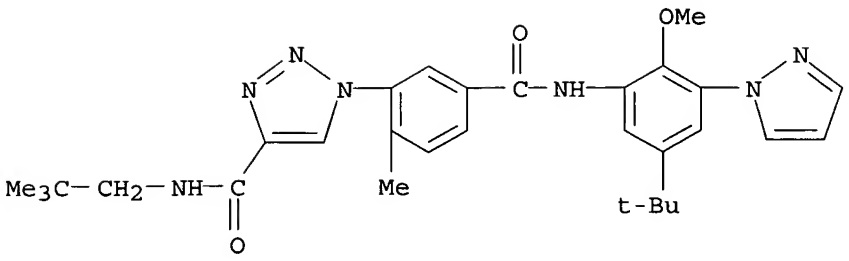
RN 855305-66-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-pyridinyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



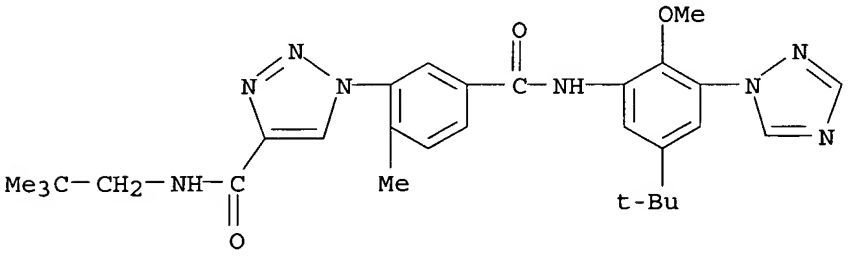
RN 855305-68-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-(1H-1,2,3-triazol-1-yl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



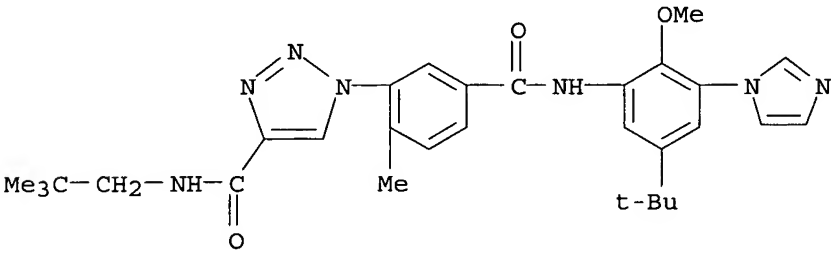
RN 855305-70-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-(1H-pyrazol-1-yl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



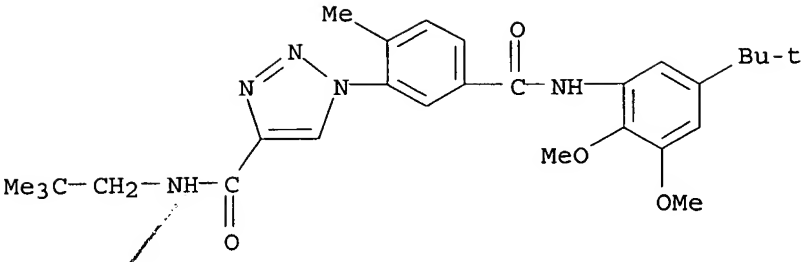
RN 855305-72-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-(1H-1,2,4-triazol-1-yl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



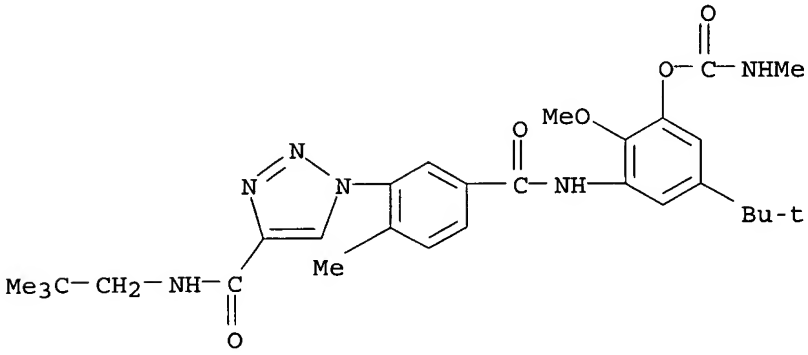
RN 855305-74-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-3-(1H-imidazol-1-yl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



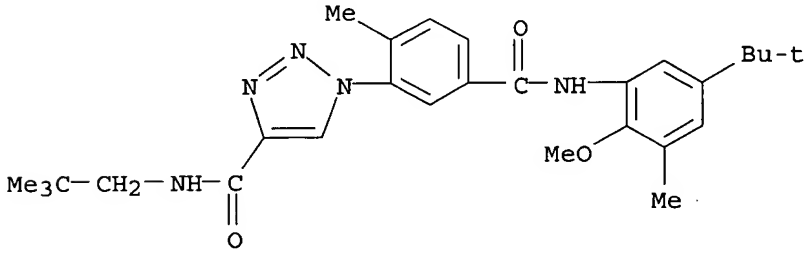
RN 855305-76-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2,3-dimethoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



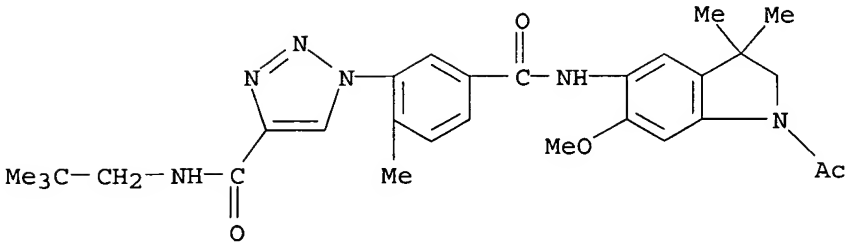
RN 855305-78-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[[(methylamino)carbonyl]oxy]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



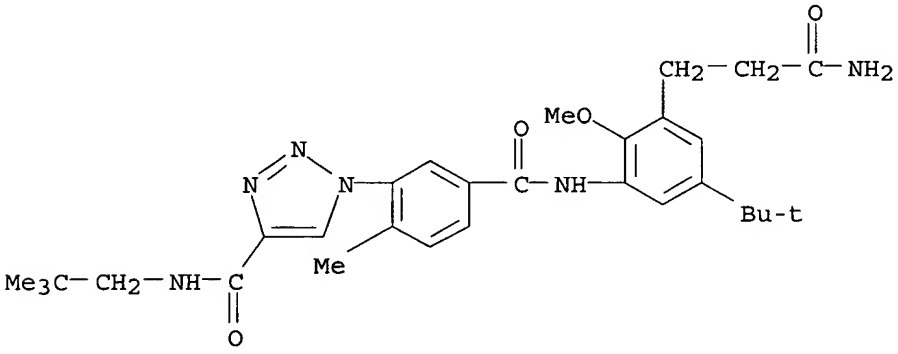
RN 855305-80-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-methylphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



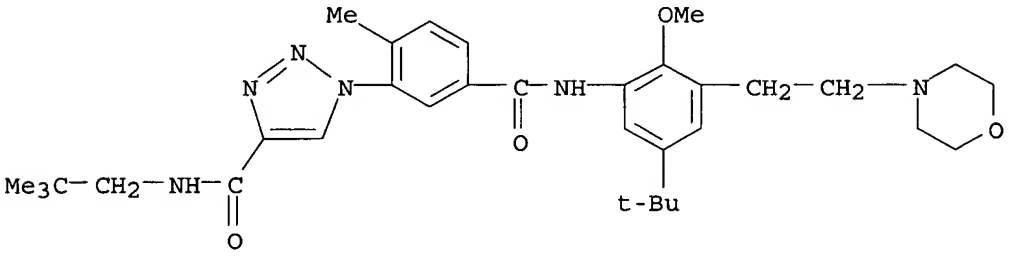
RN 855305-82-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[(1-acetyl-2,3-dihydro-6-methoxy-3,3-dimethyl-1H-indol-5-yl)amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



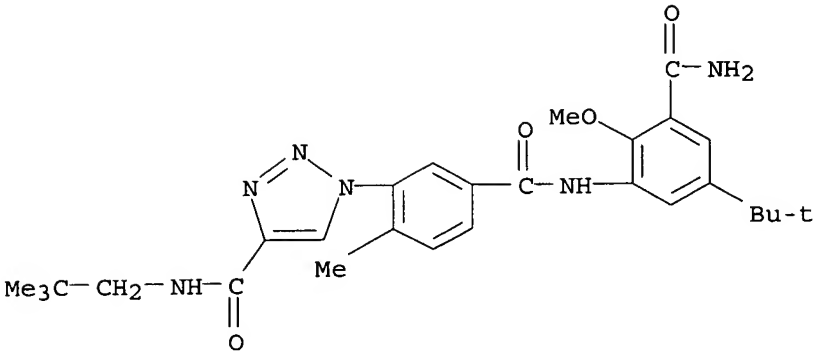
RN 855305-84-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-(3-amino-3-oxopropyl)-5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



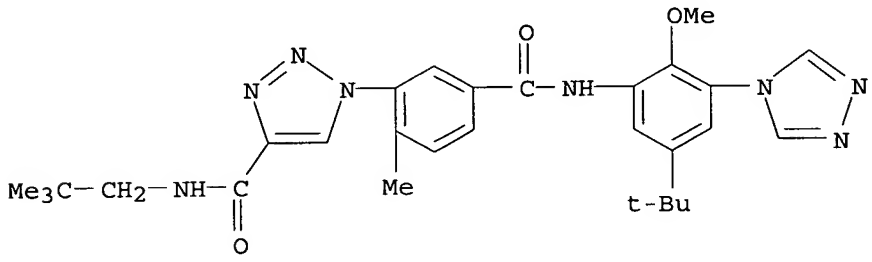
RN 855305-86-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[2-(4-morpholinyl)ethyl]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



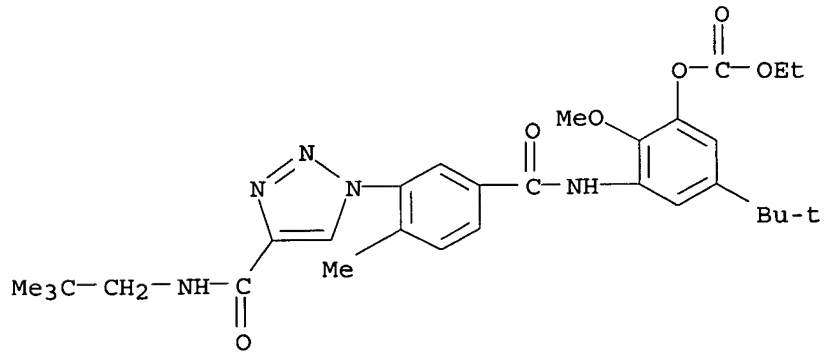
RN 855305-88-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-(aminocarbonyl)-5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



RN 855313-00-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-(4H-1,2,4-triazol-4-yl)phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



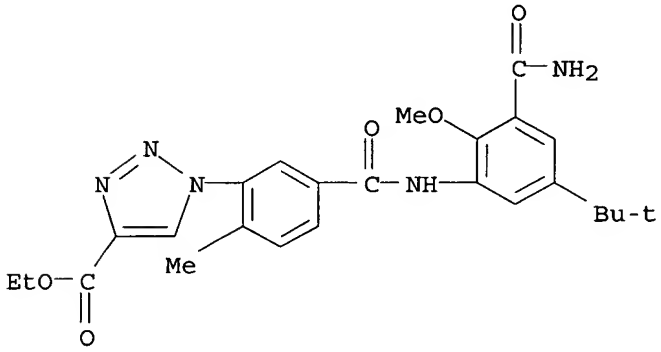
RN 855313-01-8 HCAPLUS
CN Carbonic acid, 5-(1,1-dimethylethyl)-3-[[3-[4-[[(2,2-dimethylpropyl)amino]carbonyl]-1H-1,2,3-triazol-1-yl]-4-methylbenzoyl]amino]-2-methoxyphenyl ethyl ester (9CI) (CA INDEX NAME)



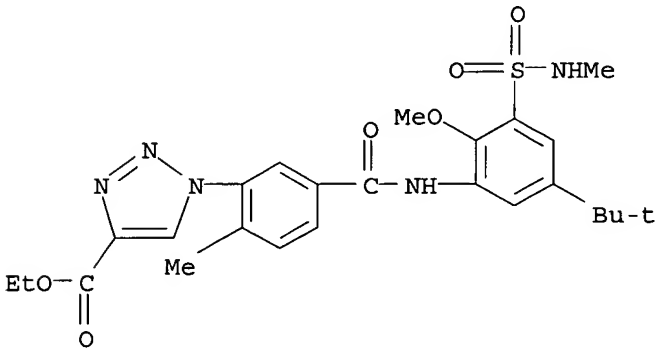
IT **855304-91-5P**, 1-[5-[(5-tert-Butyl-3-carbamoyl-2-methoxyphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid ethyl ester **855304-94-8P**, 1-[5-[(5-tert-Butyl-2-methoxy-3-methylsulfamoylphenyl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid ethyl ester **855304-96-0P**, 1-[5-[(5-tert-Butyl-2-methoxy-3-methylsulfamoylphenyl)carbamoyl]-2-methylphenyl]-1H-

[1,2,3]triazole-4-carboxylic acid **855305-16-7P**,
1-[5-[[2-(tert-Butyl)-5-methoxypyridin-4-yl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid methyl ester **855305-18-9P**,
1-[5-[(2-tert-Butyl-5-methoxypyridin-4-yl)carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid **855305-20-3P**,
1-[5-[[5-(tert-Butyl)-2-(methanesulfinyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid methyl ester **855305-22-5P**,
1-[5-[[5-tert-Butyl-2-(methanesulfinyl)phenyl]carbamoyl]-2-methylphenyl]-1H-[1,2,3]triazole-4-carboxylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2,3-triazole amide derivs. as inhibitors of cytokine production)

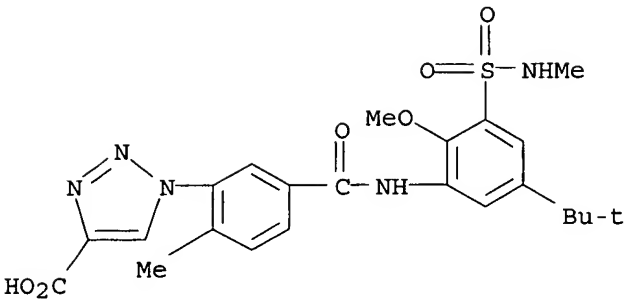
RN 855304-91-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[3-(aminocarbonyl)-5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-, ethyl ester (9CI) (CA INDEX NAME)



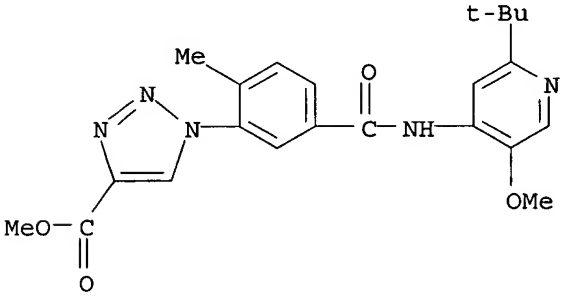
RN 855304-94-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylamino)sulfonyl]phenyl]amino]carbonyl]-2-methylphenyl]-, ethyl ester (9CI) (CA INDEX NAME)



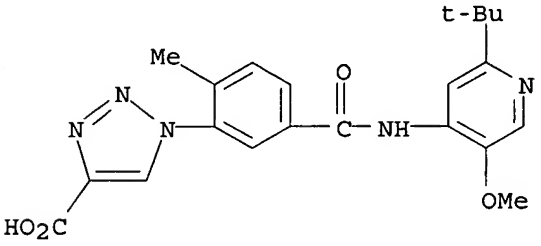
RN 855304-96-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylamino)sulfonyl]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



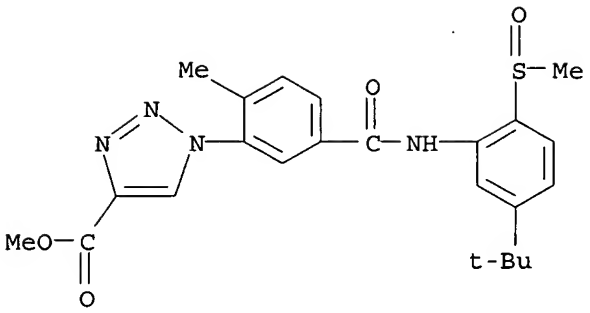
RN 855305-16-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[2-(1,1-dimethylethyl)-5-methoxy-4-pyridinyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 855305-18-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[2-(1,1-dimethylethyl)-5-methoxy-4-pyridinyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



RN 855305-20-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-(methylsulfinyl)phenyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



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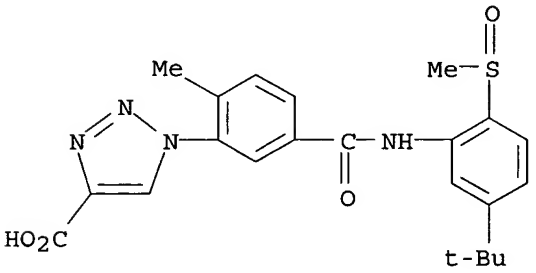
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-(methylsulfinyl)phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:433772 HCAPLUS
DOCUMENT NUMBER: 141:7121
TITLE: Preparation of aryltriazolecarboxylates as cytokine inhibitors.
INVENTOR(S): Cogan, Derek A.; Hao, Ming-Hong; Qian, Kevin Chungeng; Swinamer, Alan David
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 68 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004102492	A1	20040527	US 2003-718380	20031120
CA 2507184	AA	20040617	CA 2003-2507184	20031120
WO 2004050642	A1	20040617	WO 2003-US37104	20031120

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,

TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
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BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1567507 A1 20050831 EP 2003-789871 20031120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO.: US 2002-430519P P 20021127
WO 2003-US37104 W 20031120
OTHER SOURCE(S): CASREACT 141:7121; MARPAT 141:7121
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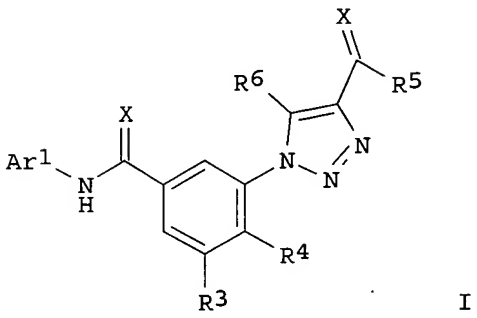


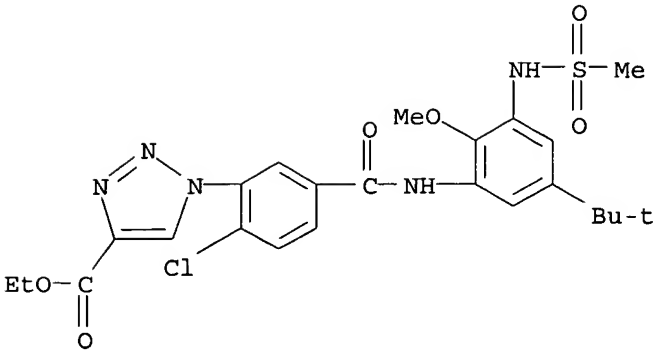
I

AB Title compds. [I; Ar1 = substituted carbocyclyl; R3, R4, R6 = H, halo, alkyl, alkoxy, OH, hydroxyalkyl, amino; R5 = bond, O, S, NH, CO, (substituted) aryl, heteroaryl, heterocyclyl; X = O, S], were prepared for treatment of osteoarthritis, atherosclerosis, contact dermatitis, bone resorption disease, etc. (no data). Thus, 1-(5-carboxy-2-methylphenyl)-1H-1,2,3-triazole-4-carboxylic acid Me ester (preparation given) was stirred with (COCl)2 and cat. DMF in CH2Cl2 to give a residue which was kept 2 h with N-(3-amino-5-tert-butyl-2-methoxyphenyl)methanesulfonamide hydrochloride and 2,6-lutidine in CH2Cl2 to give 95% 1-[5-(5-tert-butyl-3-methanesulfonylamino-2-methoxyphenylcarbamoyl)-2-methylphenyl]-1H-1,2,3-triazole-4-carboxylic acid Me ester.

IT **695178-17-7P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(claimed compound; preparation of aryltriazolecarboxylates as cytokine inhibitors)

RN 695178-17-7 HCAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



IT **695178-02-0P 695178-03-1P 695178-04-2P**
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695178-08-6P 695178-09-7P 695178-10-0P
695178-11-1P 695178-12-2P 695178-13-3P
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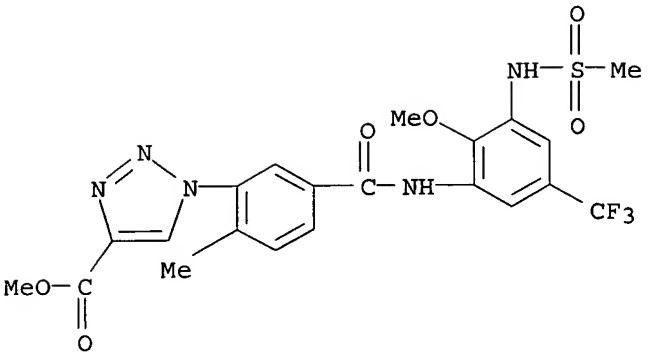
695178-79-1P 695178-80-4P 695178-81-5P
695178-82-6P 695178-83-7P 695178-84-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of aryltriazolecarboxylates as cytokine inhibitors)

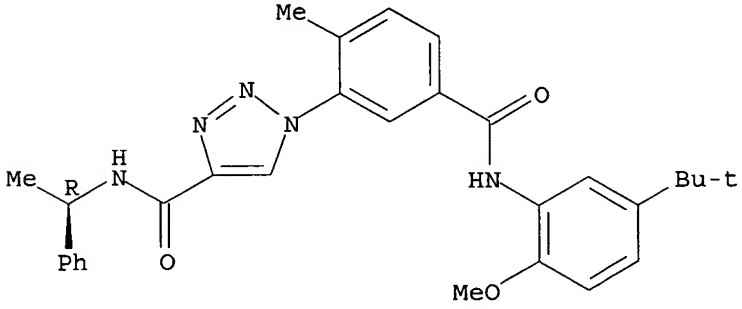
RN 695178-02-0 HCAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[2-methoxy-3-[(methylsulfonyl)amino]-5-(trifluoromethyl)phenyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)

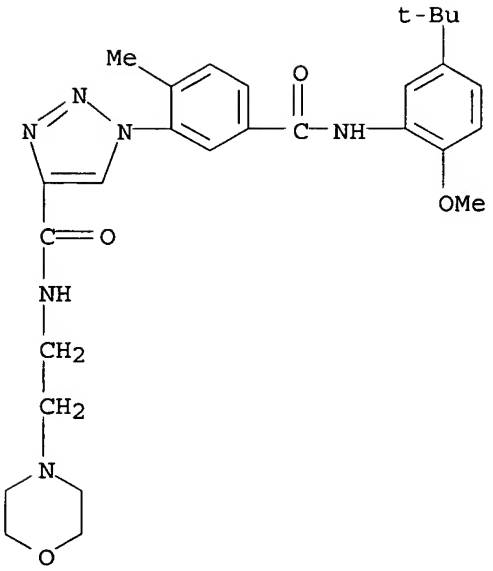


RN 695178-03-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1-phenylethyl]-(9CI) (CA INDEX NAME)

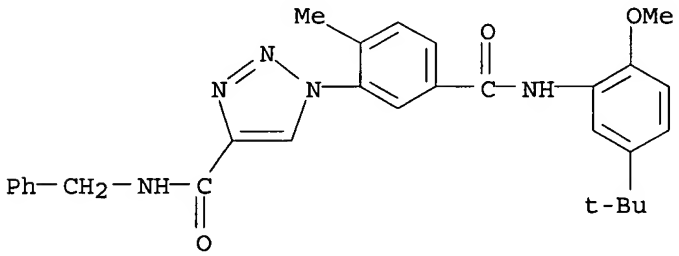
Absolute stereochemistry.



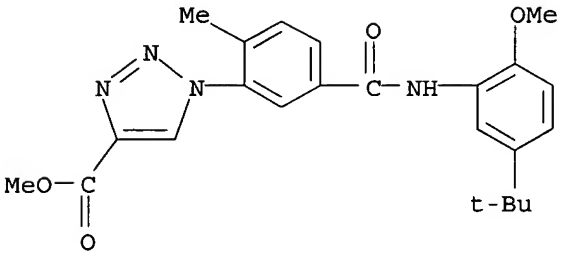
RN 695178-04-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-[2-(4-morpholinyl)ethyl]-(9CI) (CA INDEX NAME)



RN 695178-05-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



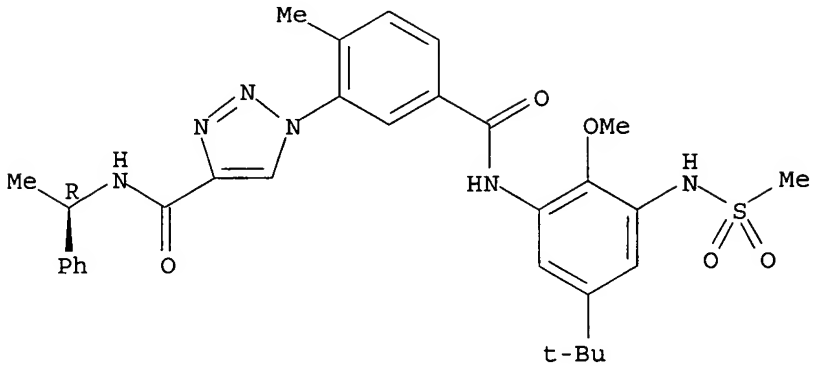
RN 695178-06-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 695178-07-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1-

phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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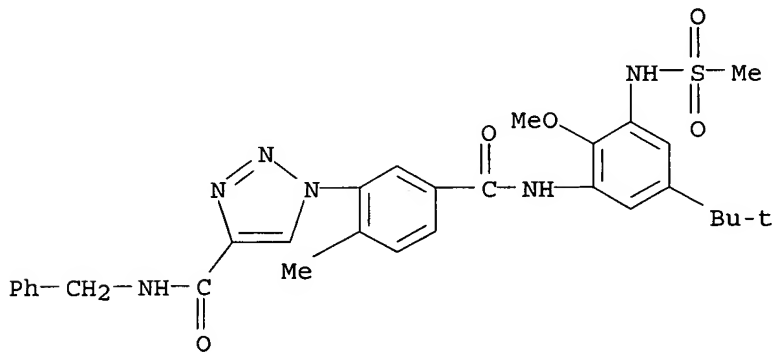
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



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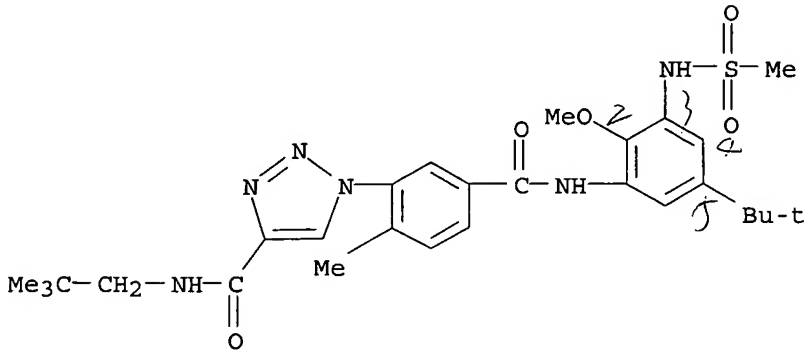
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



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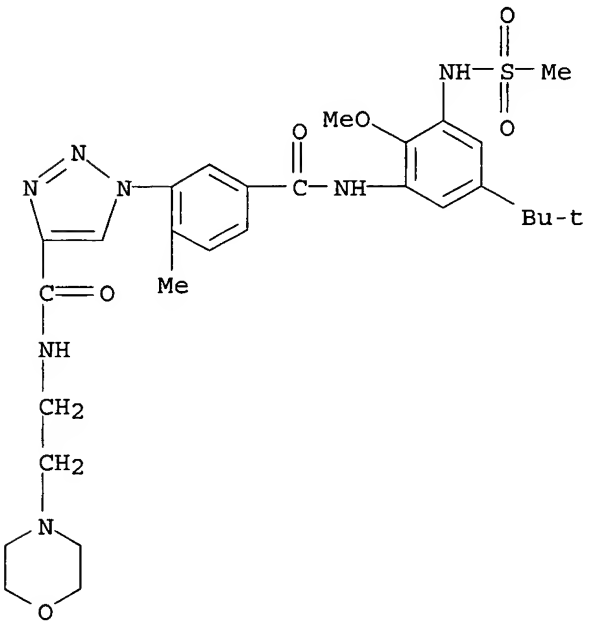
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)



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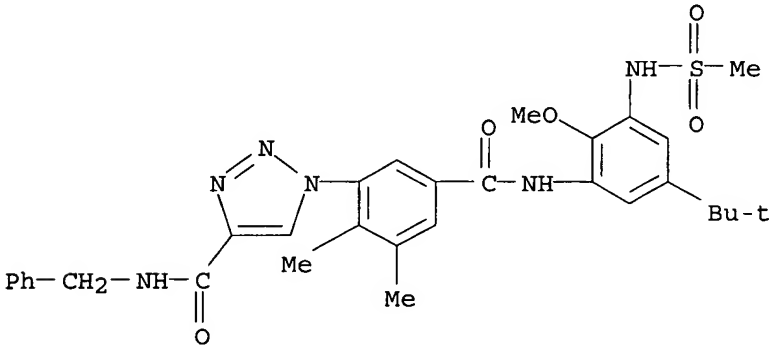
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2,3-dimethylphenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



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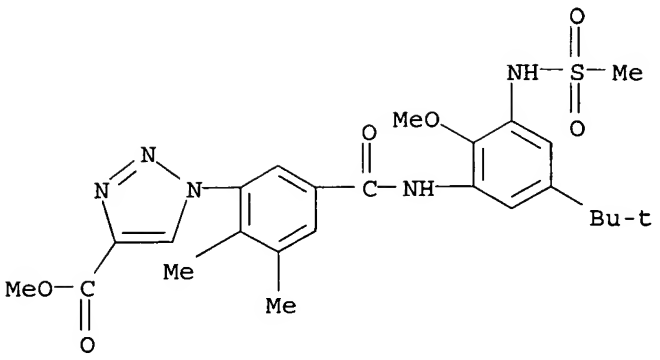
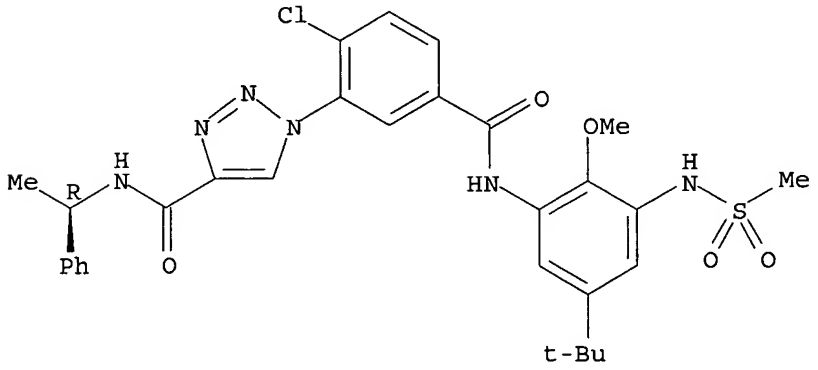
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2,3-dimethylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



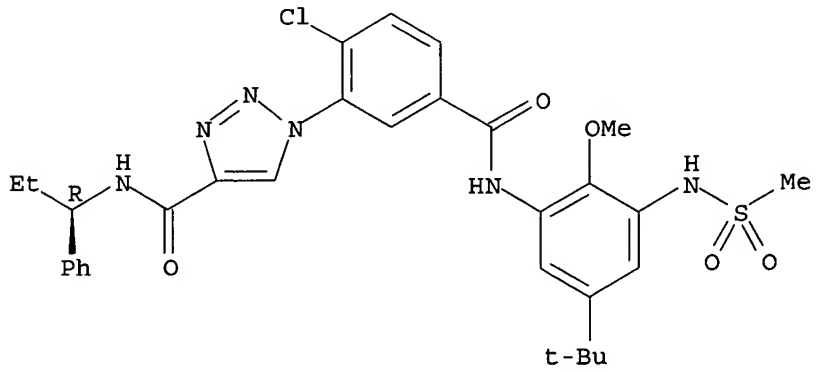
RN 695178-13-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]-N-[(1R)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 695178-14-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]-N-[(1R)-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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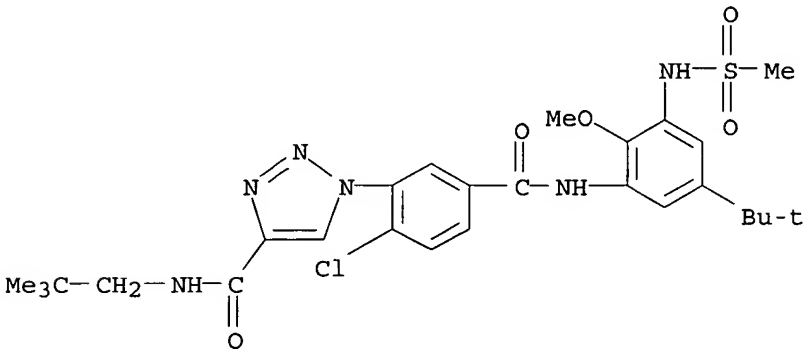

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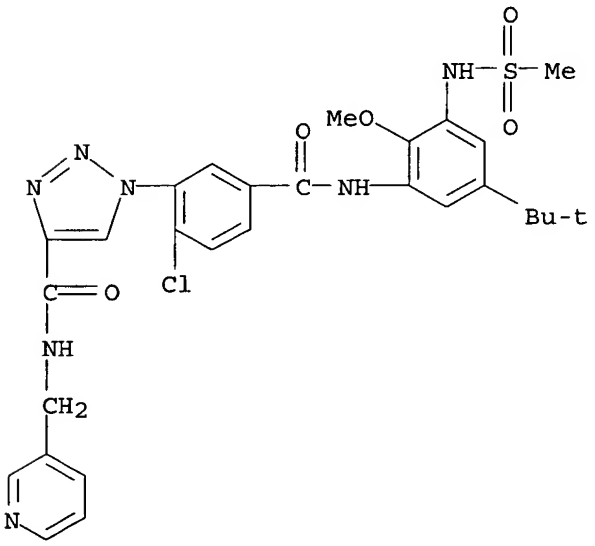
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)



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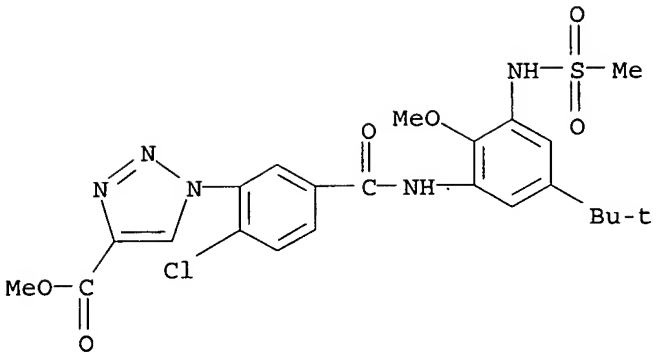
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)



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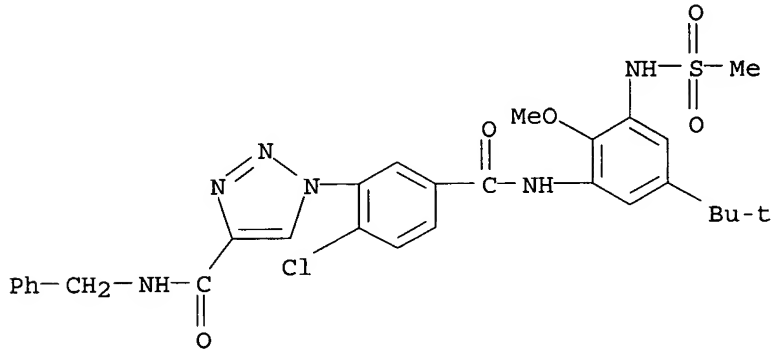
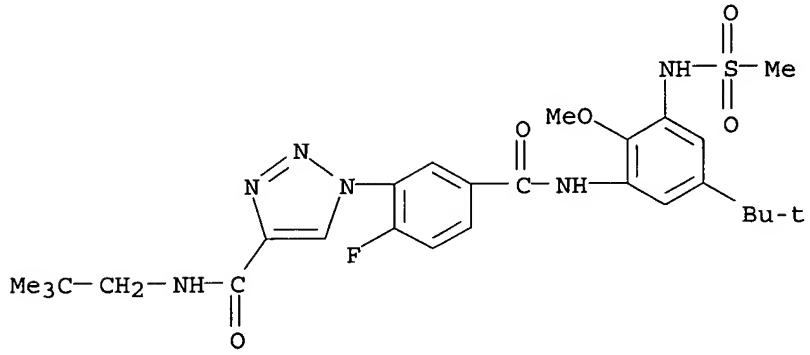
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 695178-20-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-fluorophenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



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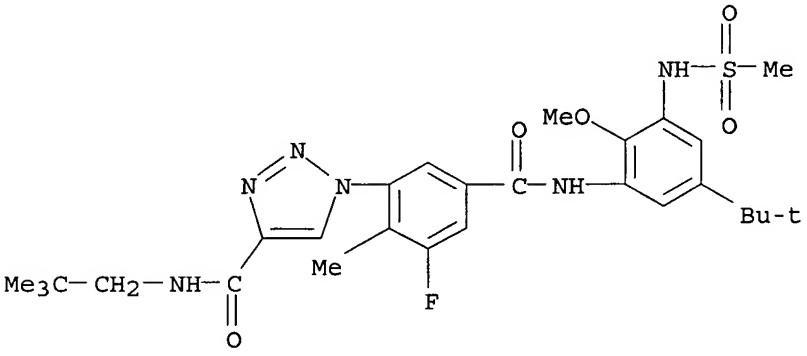
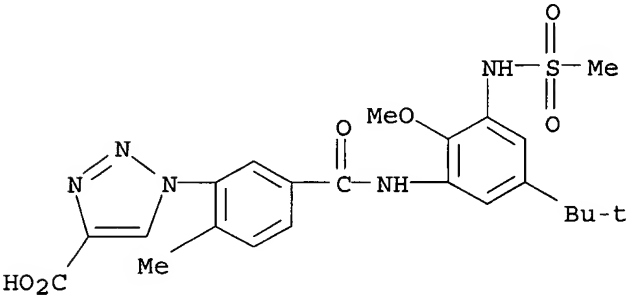
[(methylsulfonyl)amino]phenyl]amino]carbonyl]-3-fluoro-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

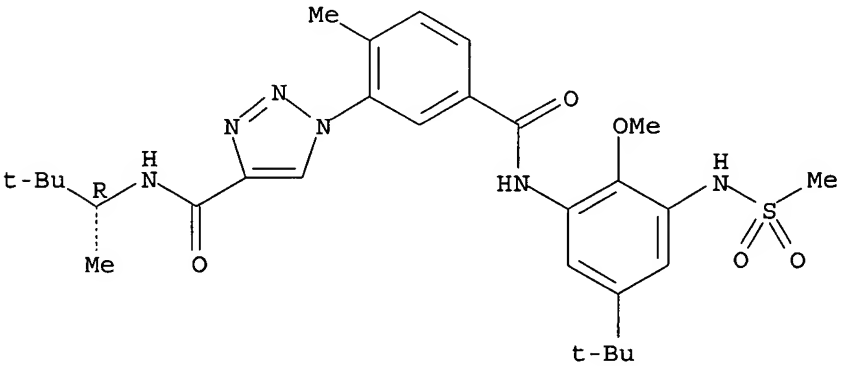


RN 695178-22-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

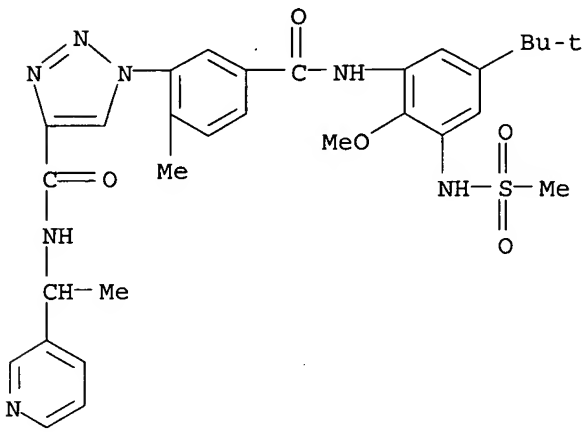


RN 695178-23-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1,2,2-trimethylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

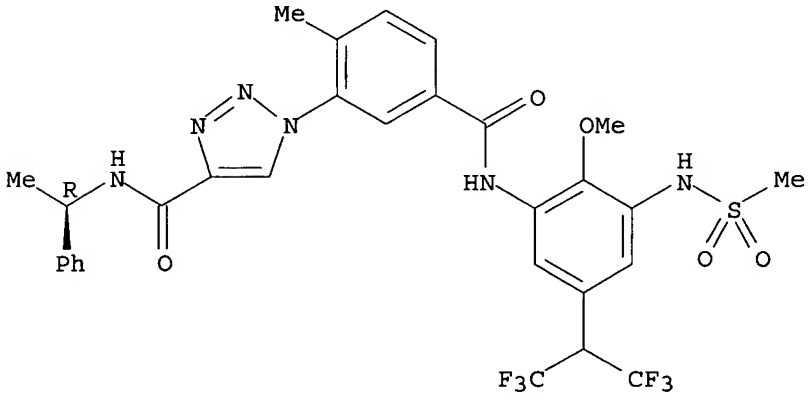


RN 695178-24-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[1-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



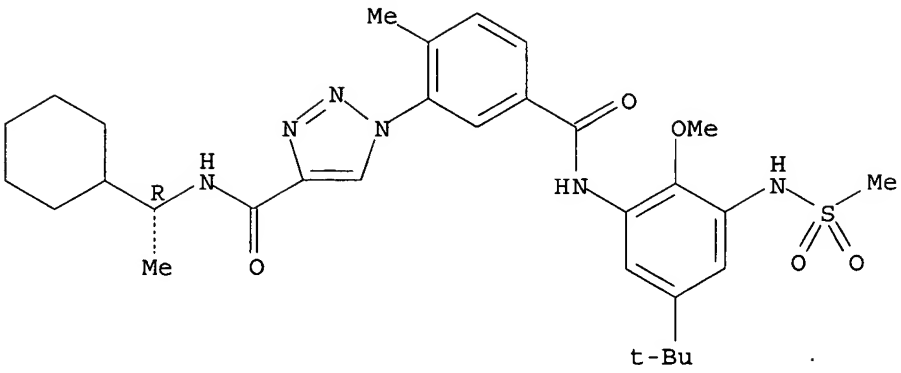
RN 695178-25-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[2-methoxy-3-[(methylsulfonyl)amino]-5-[2,2,2-trifluoro-1-(trifluoromethyl)ethyl]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



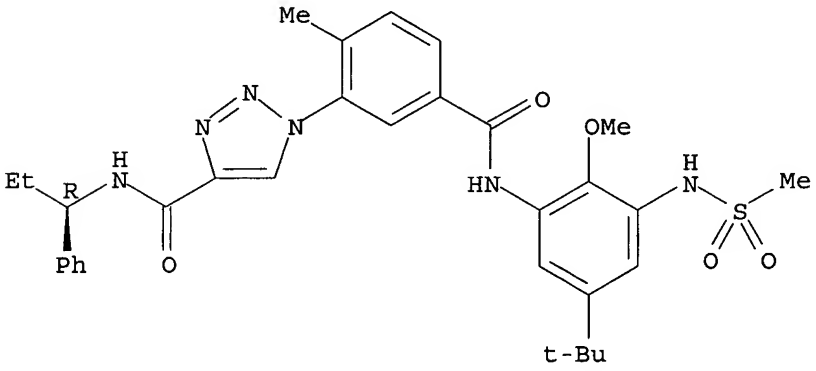
RN 695178-26-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[(1R)-1-cyclohexylethyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



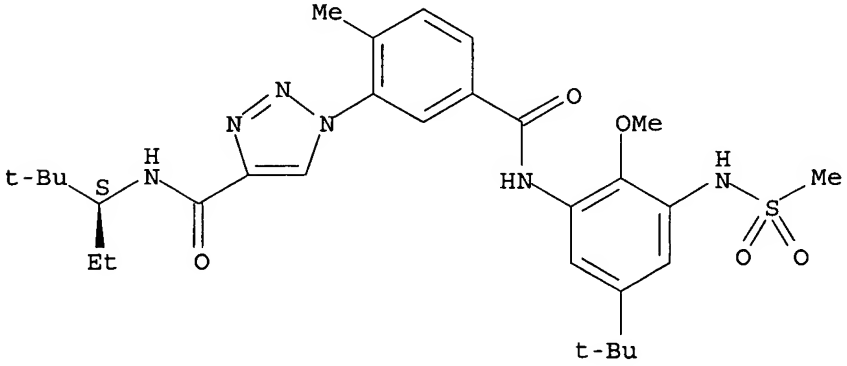
RN 695178-27-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



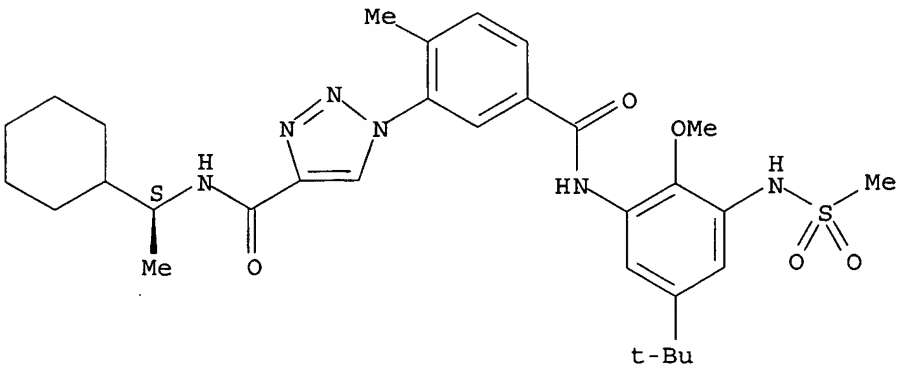
RN 695178-28-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1S)-1-ethyl-2,2-dimethylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



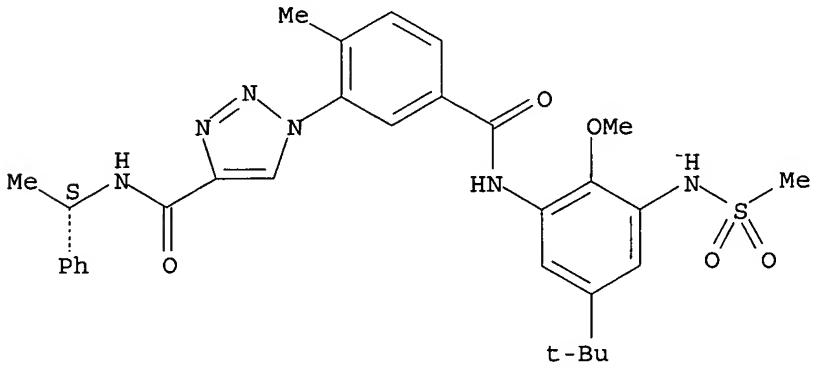
RN 695178-29-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[(1S)-1-cyclohexylethyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



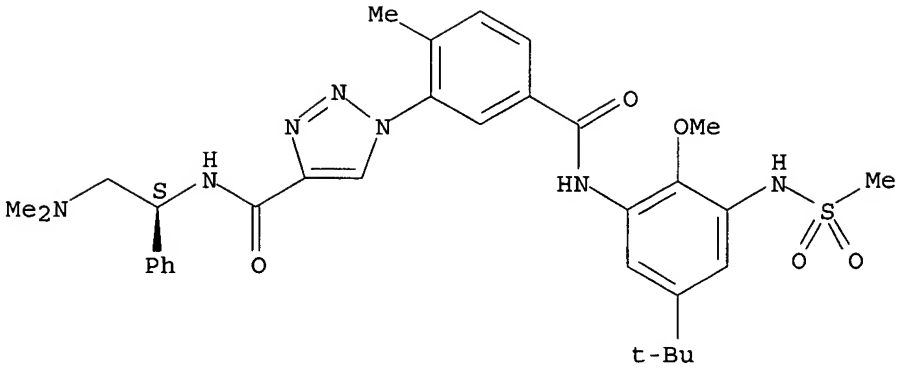
RN 695178-30-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



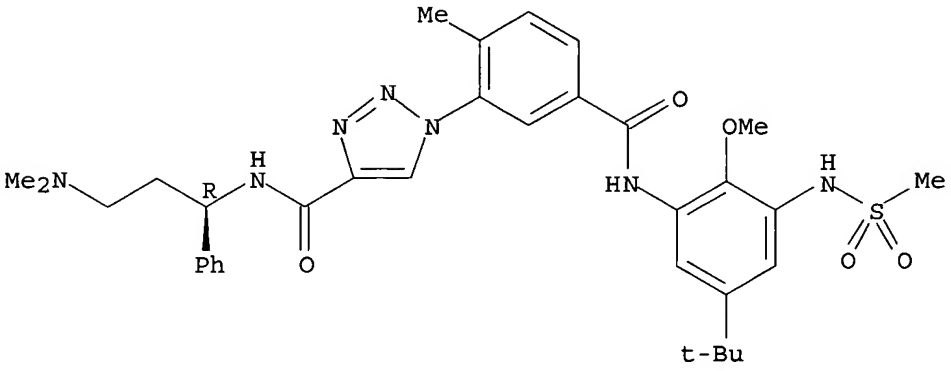
RN 695178-31-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[(1S)-2-(dimethylamino)-1-phenylethyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



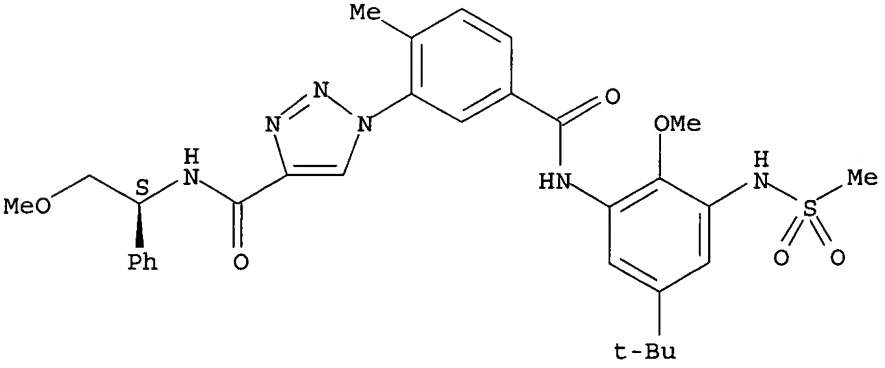
RN 695178-32-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[(1R)-3-(dimethylamino)-1-phenylpropyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

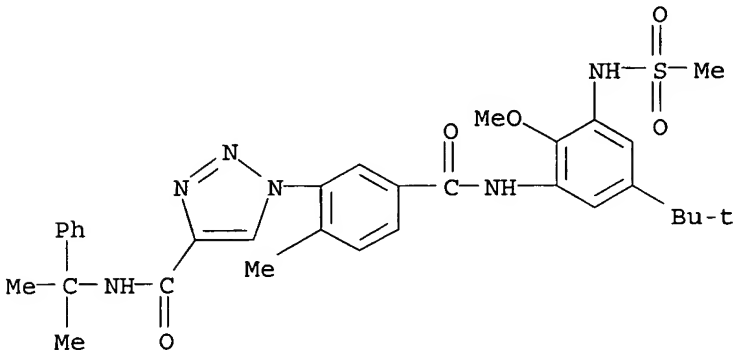


RN 695178-33-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1S)-2-methoxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

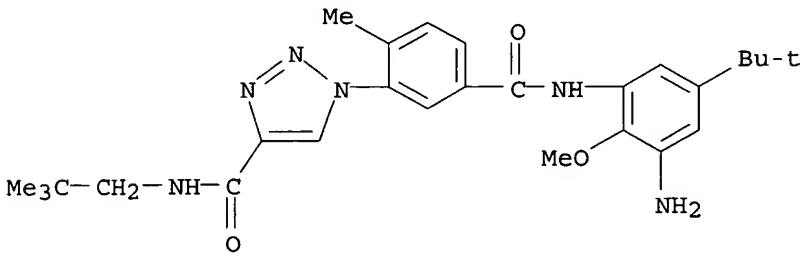
Absolute stereochemistry.



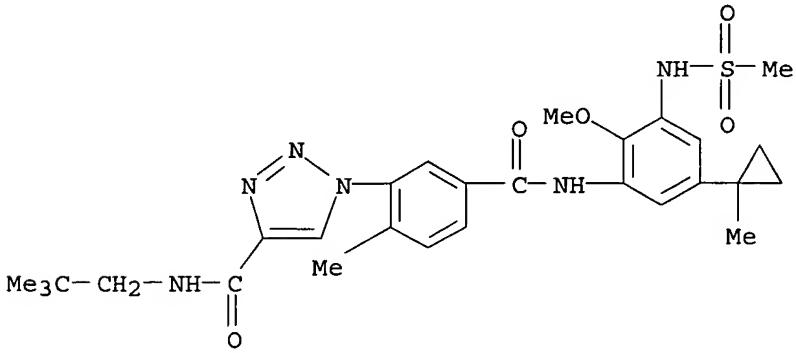
RN 695178-34-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(1-methyl-1-phenylethyl)- (9CI) (CA INDEX NAME)



RN 695178-35-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-amino-5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)

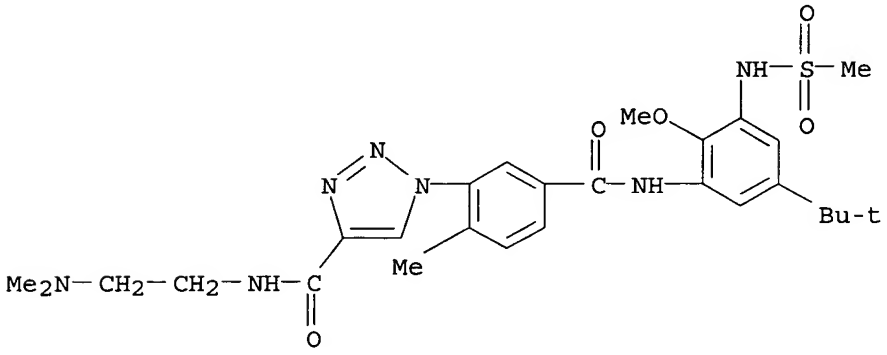


RN 695178-37-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-(2,2-dimethylpropyl)-1-[5-[[[2-methoxy-5-(1-methylcyclopropyl)-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

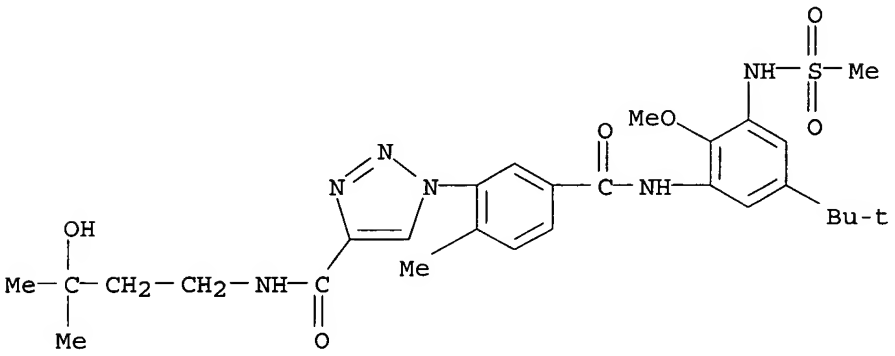


RN 695178-38-2 HCAPLUS

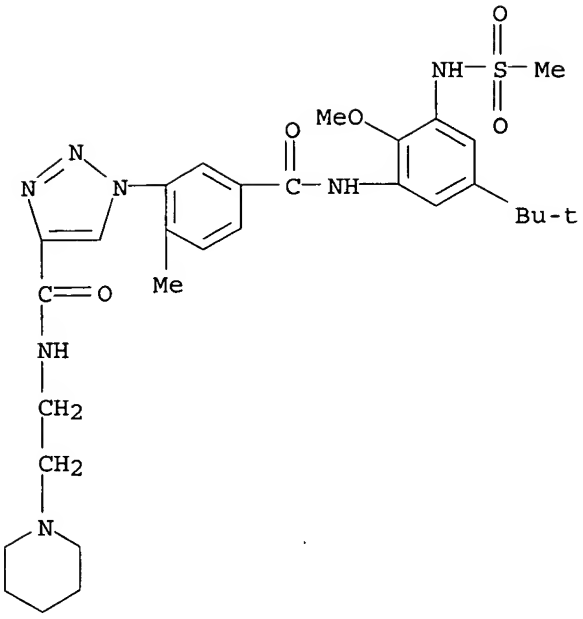
CN 1H-1,2,3-Triazole-4-carboxamide, N-[2-(dimethylamino)ethyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



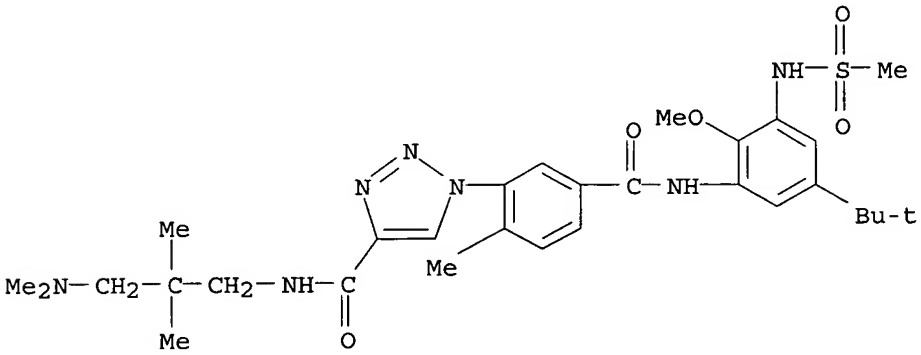
RN 695178-39-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(3-hydroxy-3-methylbutyl)- (9CI) (CA INDEX NAME)



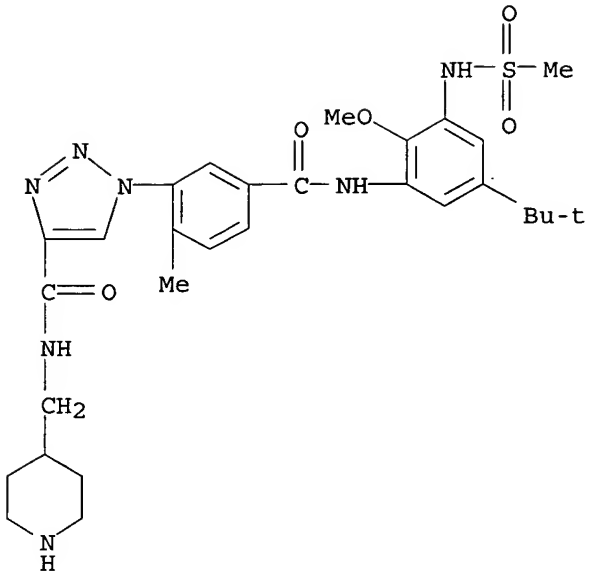
RN 695178-40-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



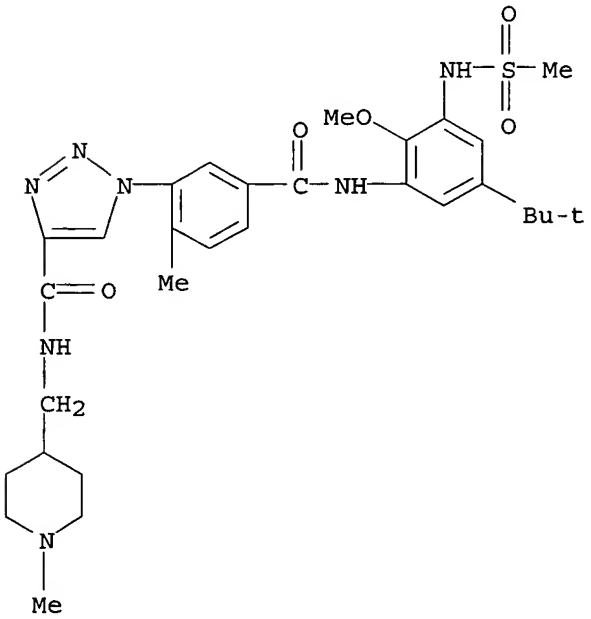
RN 695178-41-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[3-(dimethylamino)-2,2-dimethylpropyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



RN 695178-42-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(4-piperidinylmethyl)- (9CI) (CA INDEX NAME)

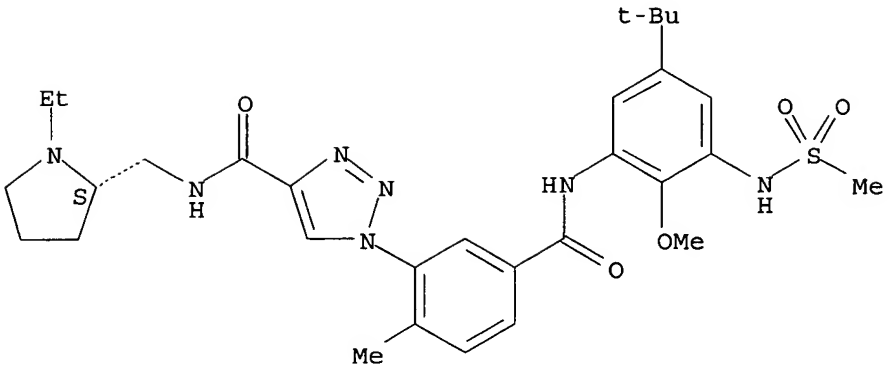


RN 695178-43-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1-methyl-4-piperidinyl)methyl]- (9CI) (CA INDEX NAME)



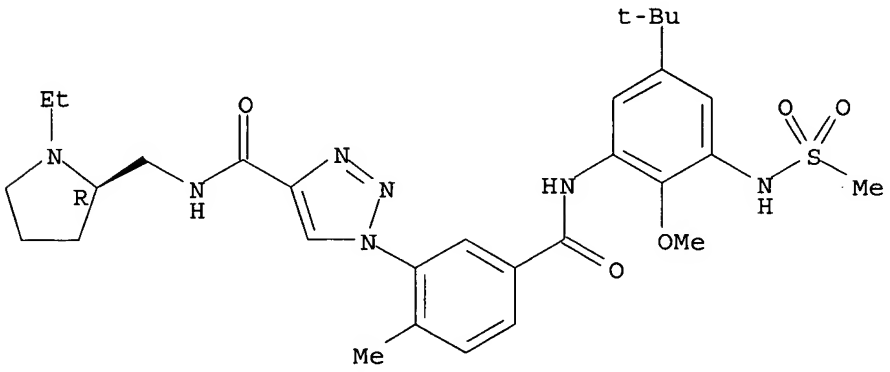
RN 695178-44-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[[(2S)-1-ethyl-2-pyrrolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

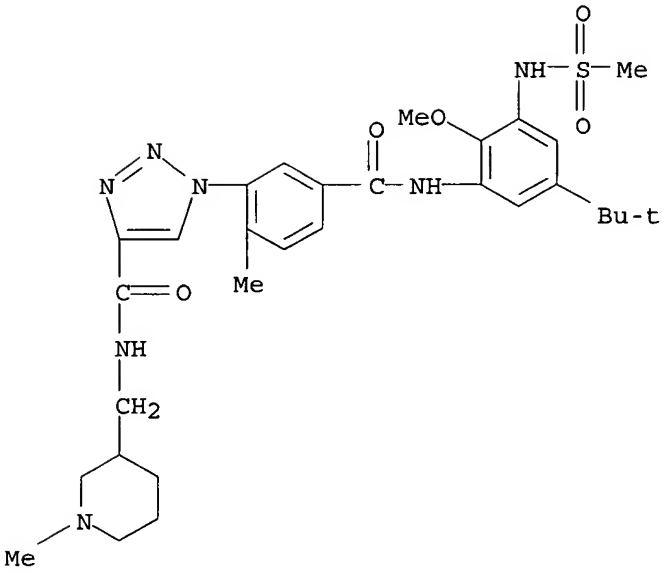


RN 695178-45-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[[(2R)-1-ethyl-2-pyrrolidinyl]methyl]- (9CI) (CA INDEX NAME)

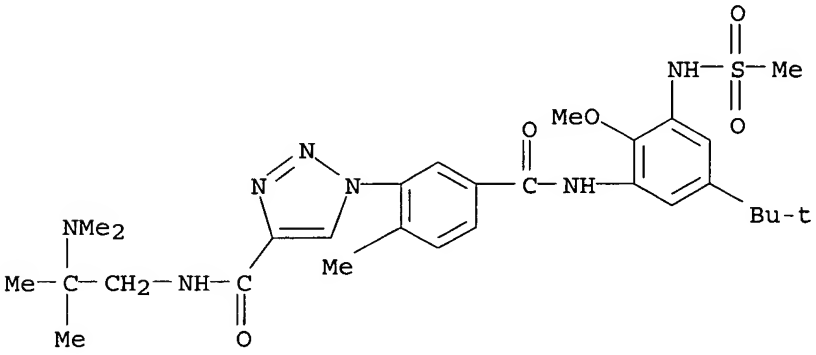
Absolute stereochemistry.



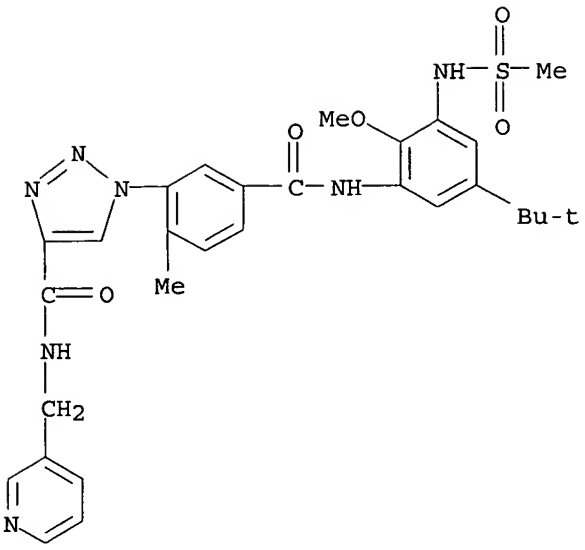
RN 695178-46-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1-methyl-3-piperidinyl)methyl]- (9CI) (CA INDEX NAME)



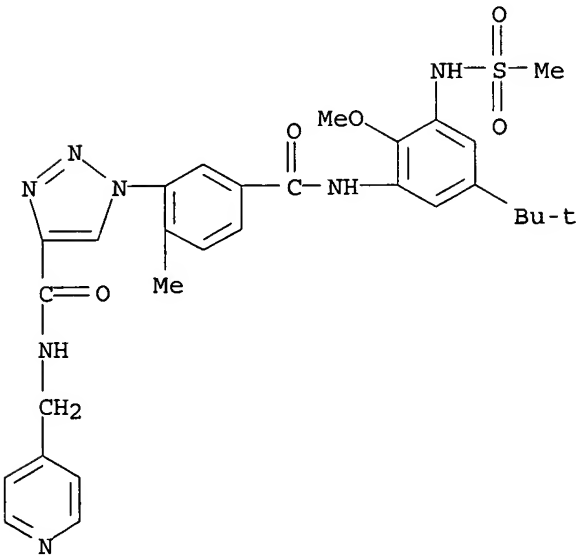
RN 695178-47-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[2-(dimethylamino)-2-methylpropyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



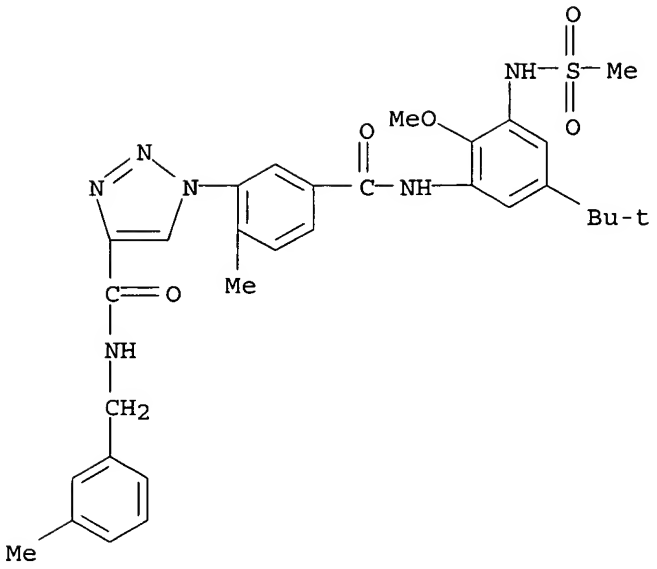
RN 695178-48-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)



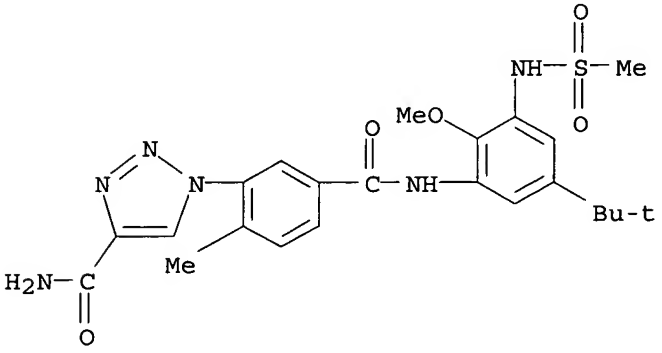
RN 695178-49-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



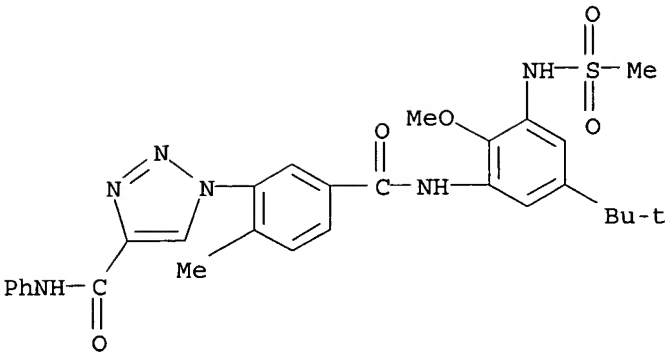
RN 695178-50-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



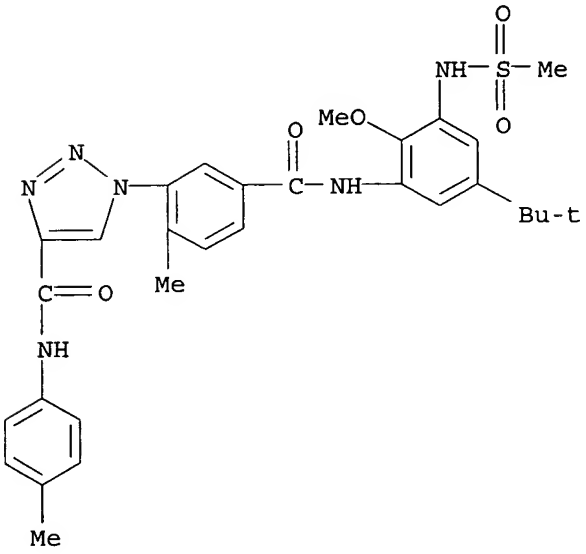
RN 695178-51-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



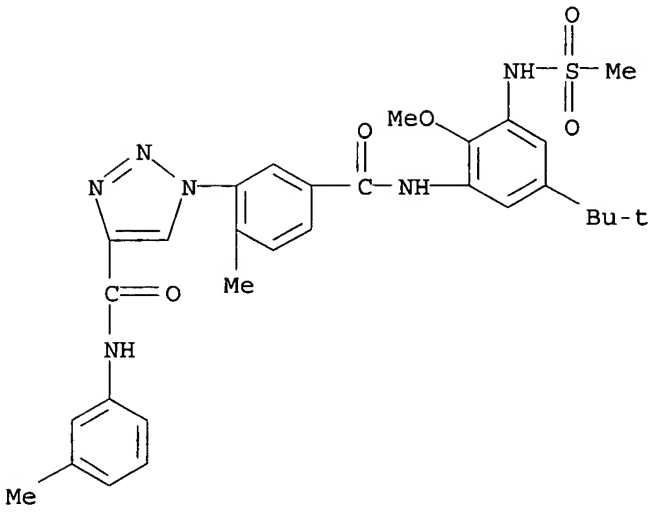
RN 695178-52-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-phenyl- (9CI) (CA INDEX NAME)



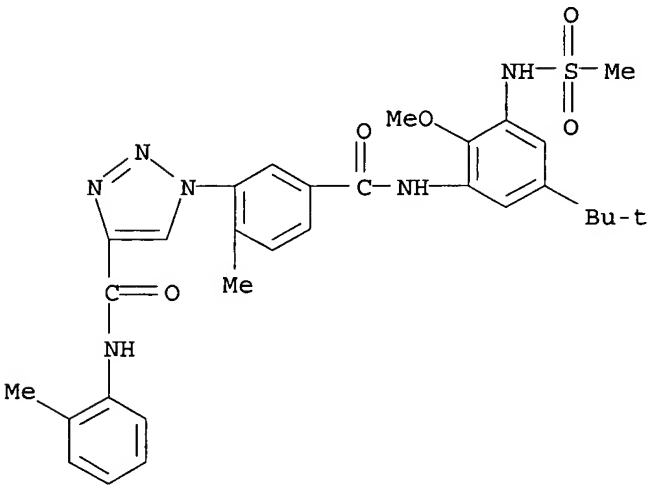
RN 695178-53-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(4-methylphenyl)- (9CI) (CA INDEX NAME)



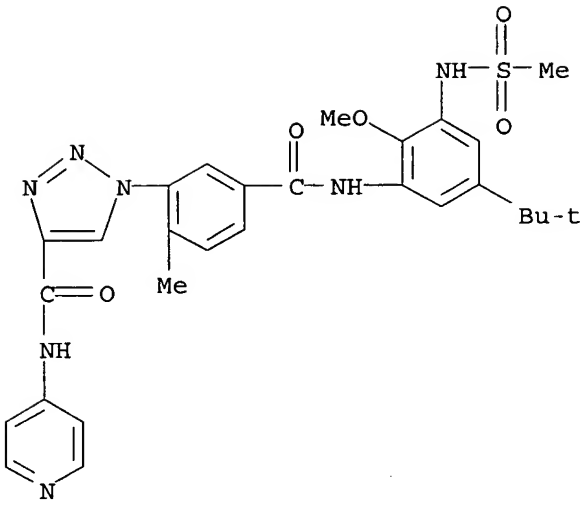
RN 695178-54-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(3-methylphenyl)- (9CI) (CA INDEX NAME)



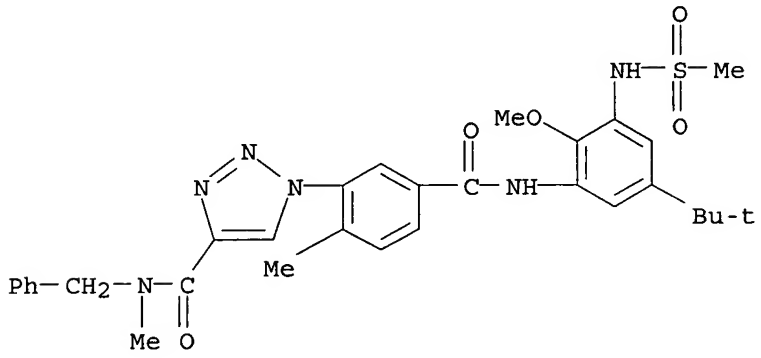
RN 695178-55-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2-methylphenyl)- (9CI) (CA INDEX NAME)



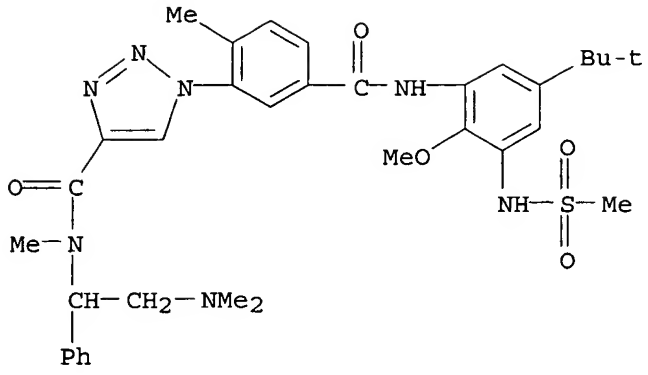
RN 695178-56-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-4-pyridinyl- (9CI) (CA INDEX NAME)



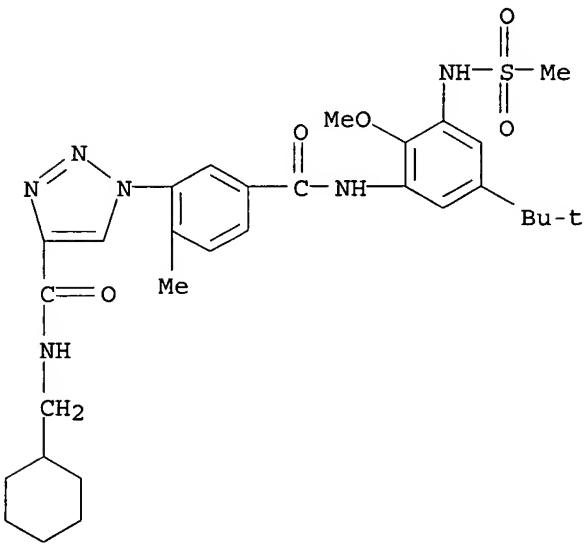
RN 695178-57-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



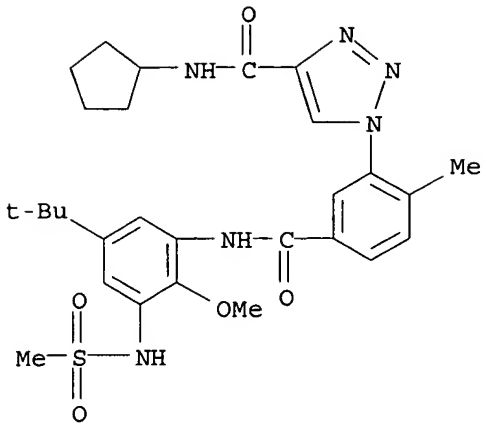
RN 695178-58-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-[2-(dimethylamino)-1-phenylethyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-methyl- (9CI) (CA INDEX NAME)



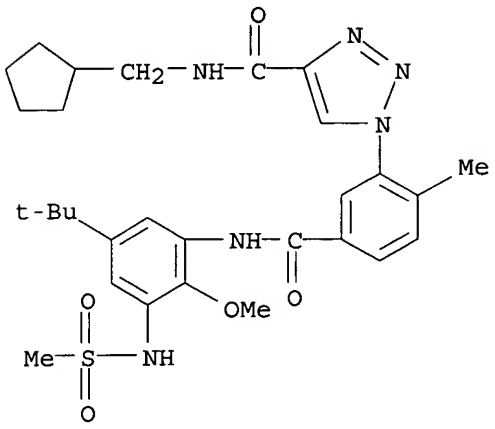
RN 695178-59-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-(cyclohexylmethyl)-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



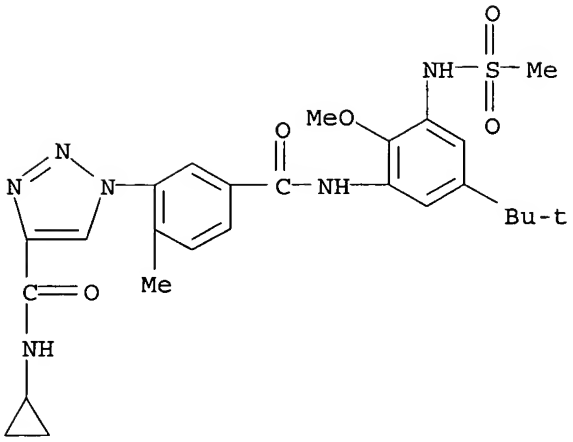
RN 695178-60-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-cyclopentyl-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



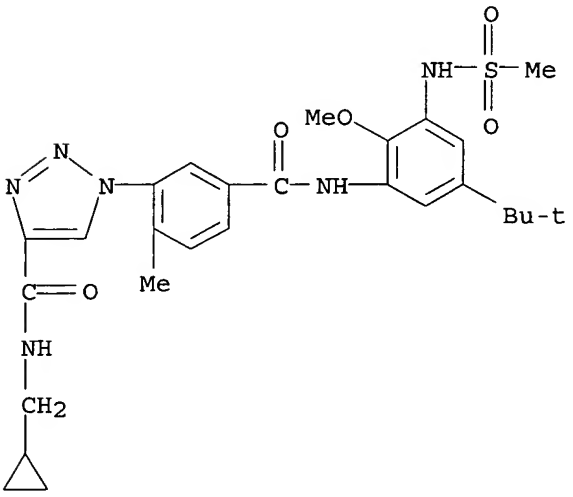
RN 695178-61-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-(cyclopentylmethyl)-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



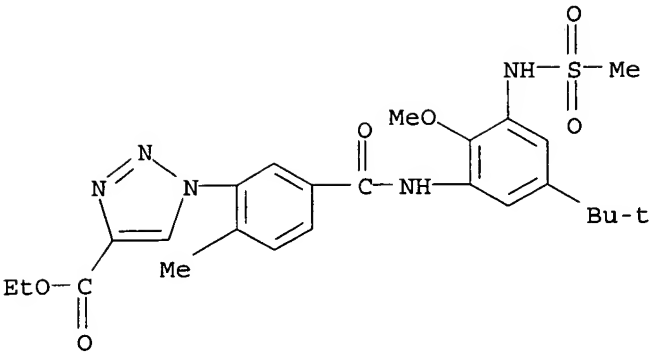
RN 695178-62-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-cyclopropyl-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



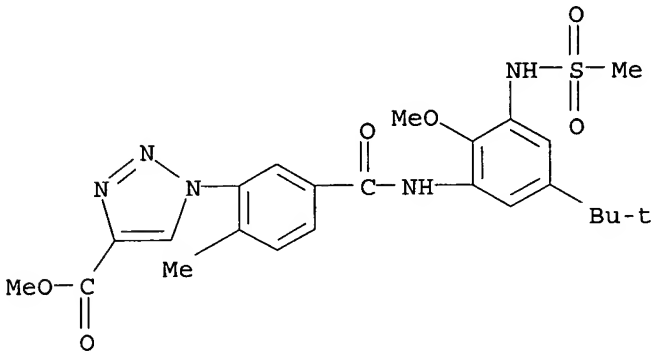
RN 695178-63-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-(cyclopropylmethyl)-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



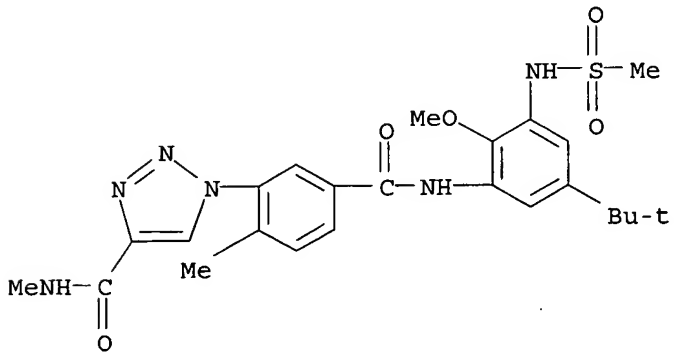
RN 695178-64-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 695178-65-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)

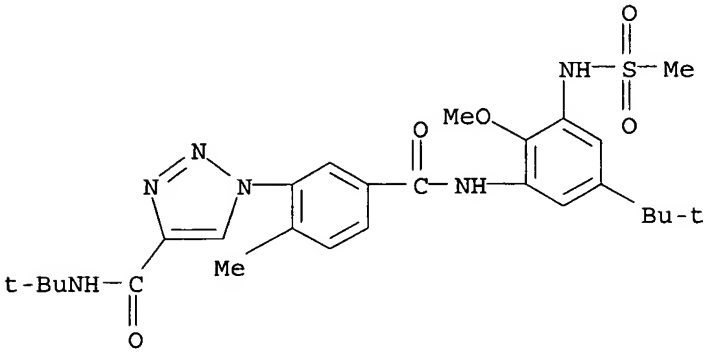


RN 695178-66-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-methyl- (9CI) (CA INDEX NAME)

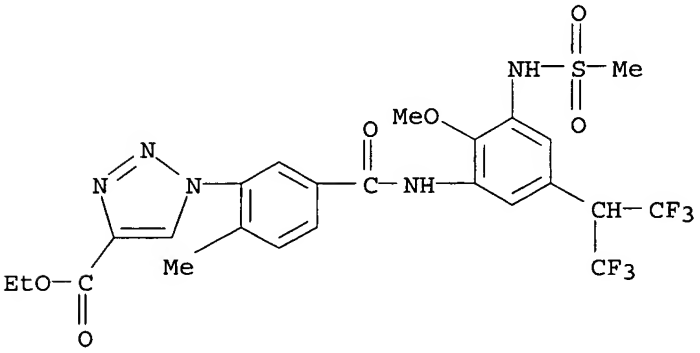


RN 695178-67-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, N-(1,1-dimethylethyl)-1-[5-[[[5-(1,1-

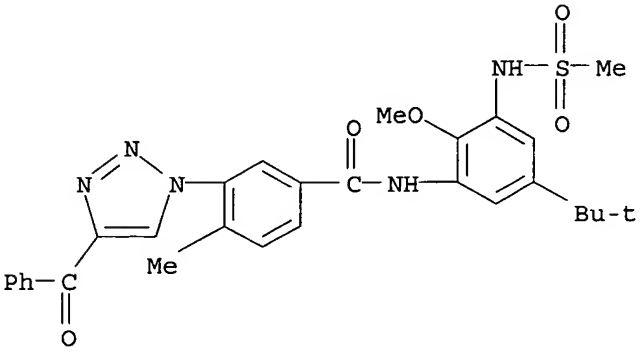
dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



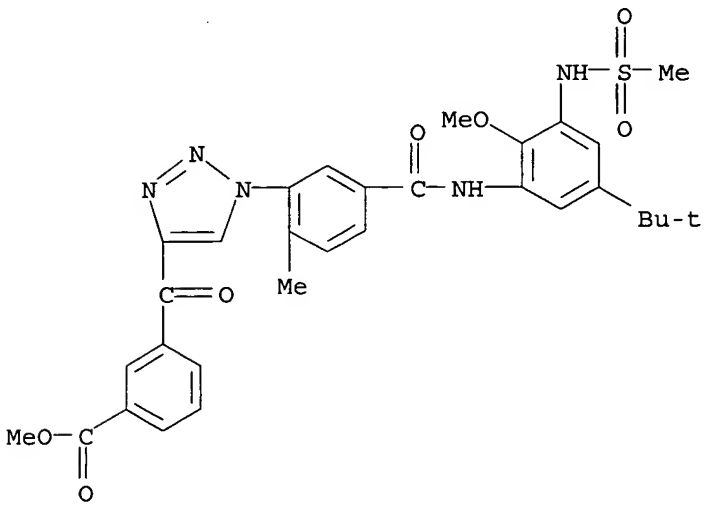
RN 695178-68-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[2-methoxy-3-[(methylsulfonyl)amino]-5-[2,2,2-trifluoro-1-(trifluoromethyl)ethyl]phenyl]amino]carbonyl]-2-methylphenyl]-, ethyl ester (9CI) (CA INDEX NAME)



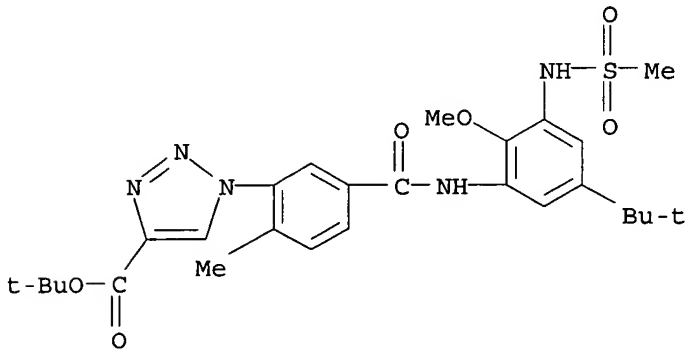
RN 695178-69-9 HCAPLUS
CN Benzamide, 3-(4-benzoyl-1H-1,2,3-triazol-1-yl)-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)



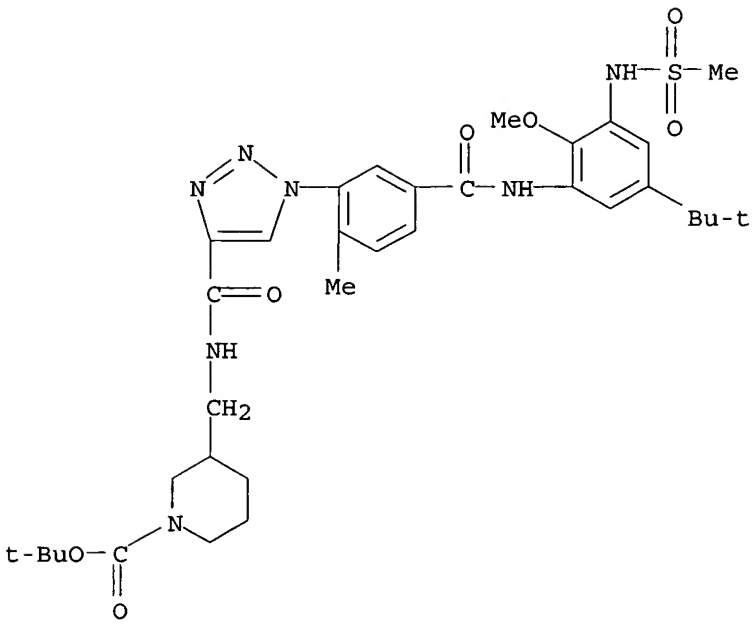
RN 695178-70-2 HCAPLUS
CN Benzoic acid, 3-[[1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-1H-1,2,3-triazol-4-yl]carbonyl]-, methyl ester (9CI) (CA INDEX NAME)



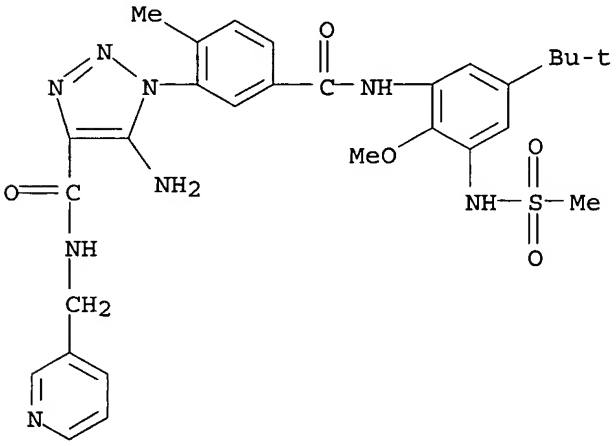
RN 695178-71-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 695178-72-4 HCAPLUS
CN 1-Piperidinecarboxylic acid, 3-[[[[1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-1H-1,2,3-triazol-4-yl]carbonyl]amino]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

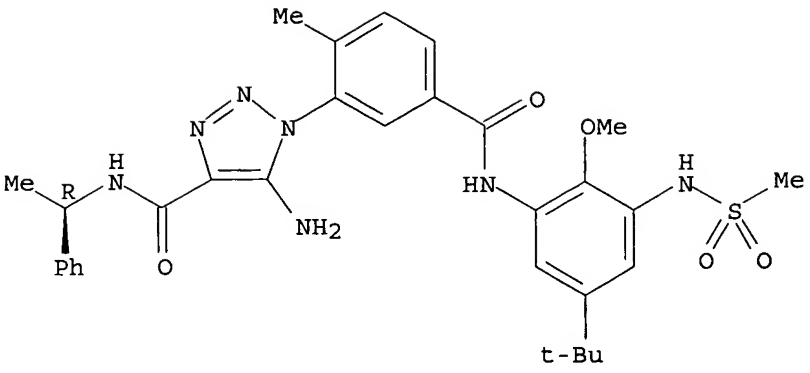


RN 695178-73-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 5-amino-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

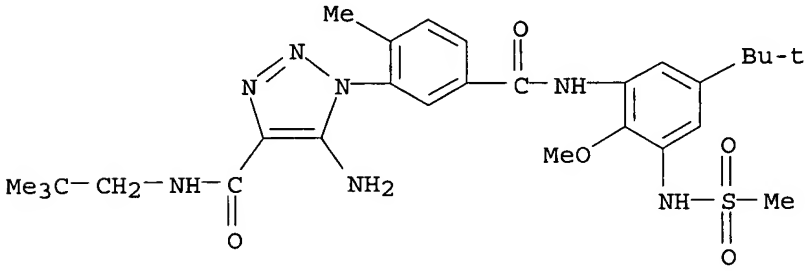


RN 695178-74-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 5-amino-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1R)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

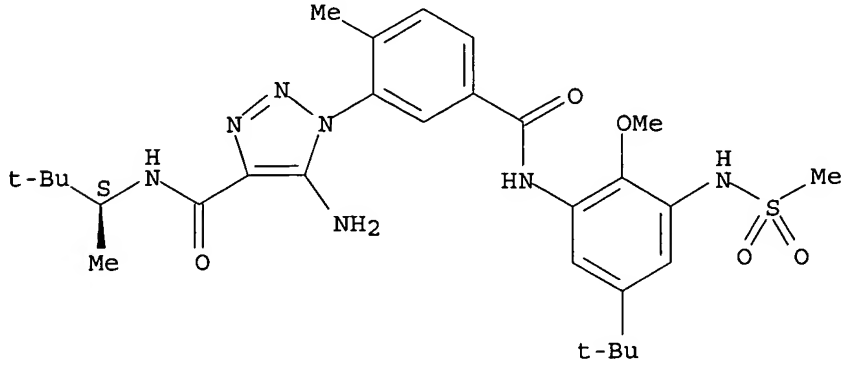


RN 695178-75-7 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 5-amino-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



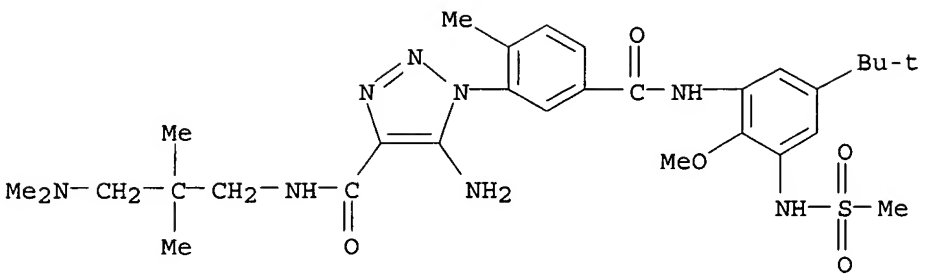
RN 695178-76-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 5-amino-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1S)-1,2,2-trimethylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

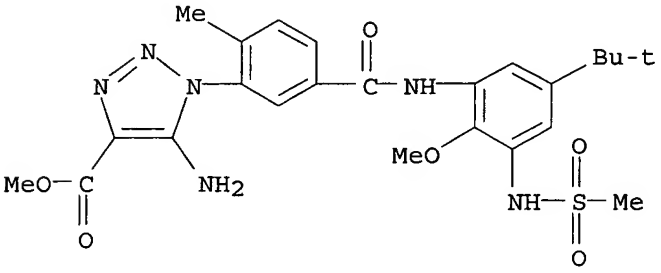


RN 695178-77-9 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 5-amino-N-[3-(dimethylamino)-2,2-dimethylpropyl]-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA

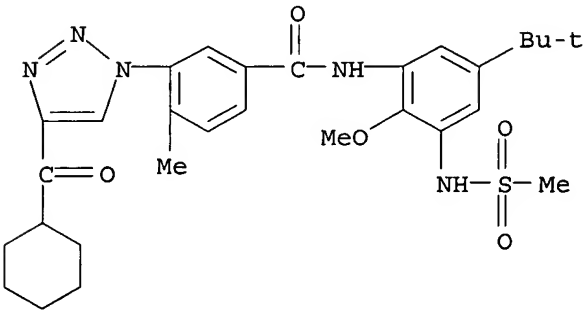
INDEX NAME)



RN 695178-78-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-amino-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)

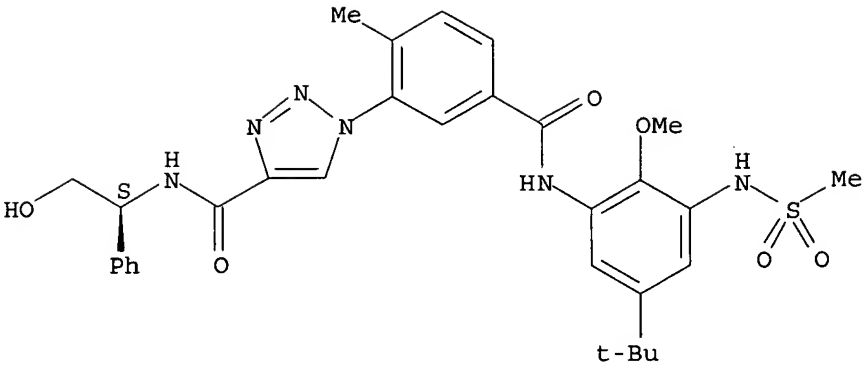


RN 695178-79-1 HCAPLUS
CN Benzamide, 3-[4-(cyclohexylcarbonyl)-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)

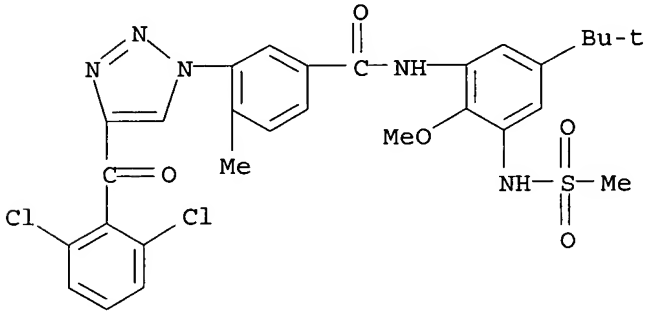


RN 695178-80-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

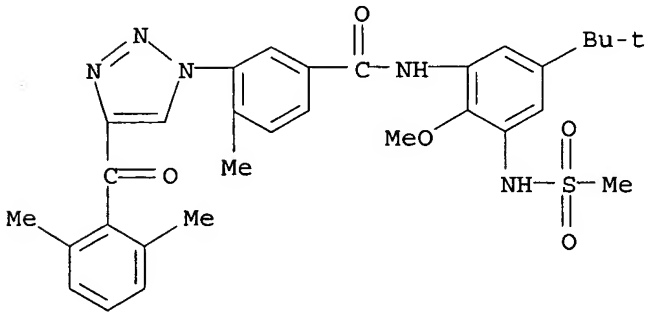
Absolute stereochemistry.



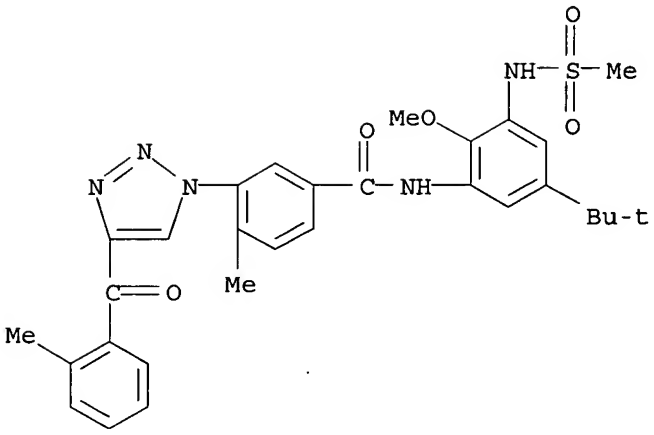
RN 695178-81-5 HCAPLUS
CN Benzamide, 3-[4-(2,6-dichlorobenzoyl)-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)



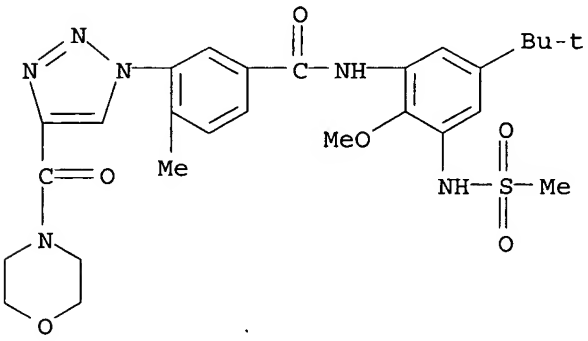
RN 695178-82-6 HCAPLUS
CN Benzamide, 3-[4-(2,6-dimethylbenzoyl)-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (9CI) (CA INDEX NAME)



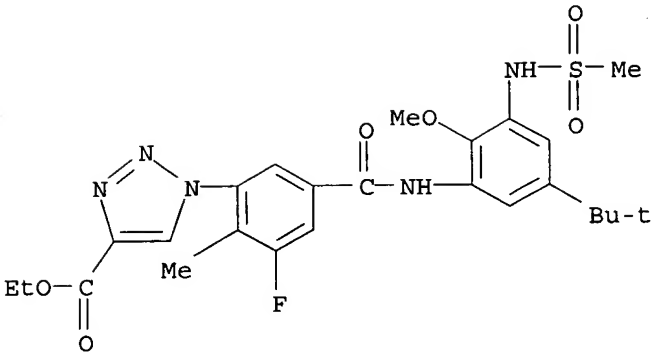
RN 695178-83-7 HCAPLUS
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(2-methylbenzoyl)-1H-1,2,3-triazol-1-yl]- (9CI) (CA INDEX NAME)



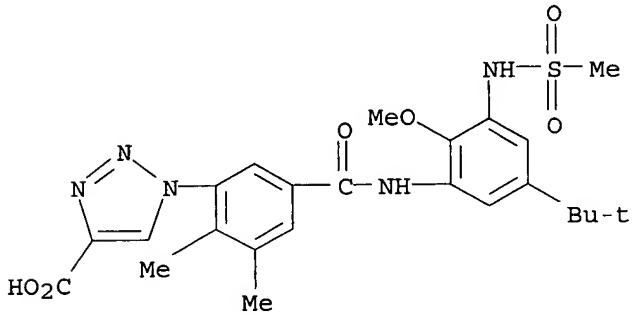
RN 695178-84-8 HCAPLUS
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(4-morpholinylcarbonyl)-1H-1,2,3-triazol-1-yl]- (9CI) (CA INDEX NAME)



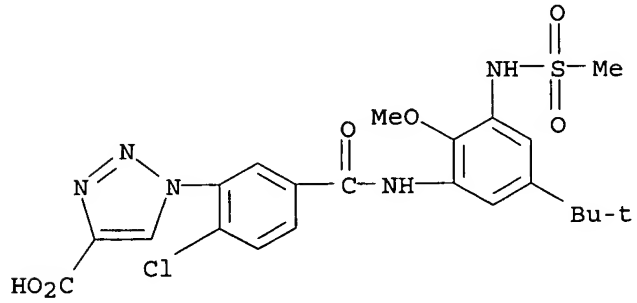
IT **695178-92-8P 695178-96-2P 695178-97-3P**
695178-98-4P 695178-99-5P 695179-02-3P
695179-03-4P 695179-04-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryltriazolecarboxylates as cytokine inhibitors)
RN 695178-92-8 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-3-fluoro-2-methylphenyl]-, ethyl ester (9CI) (CA INDEX NAME)



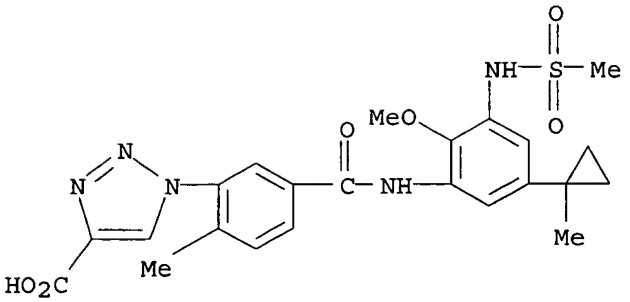
RN 695178-96-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2,3-dimethylphenyl]- (9CI) (CA INDEX NAME)



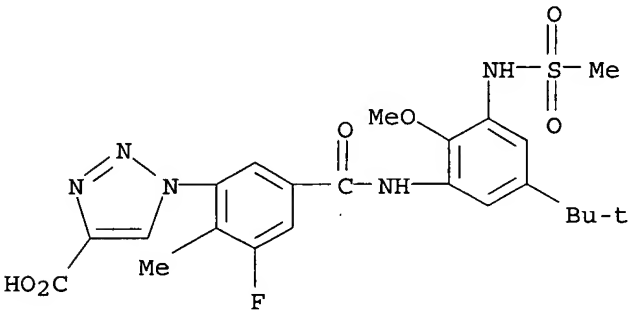
RN 695178-97-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[2-chloro-5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]phenyl]- (9CI) (CA INDEX NAME)



RN 695178-98-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[2-methoxy-5-(1-methylcyclopropyl)-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

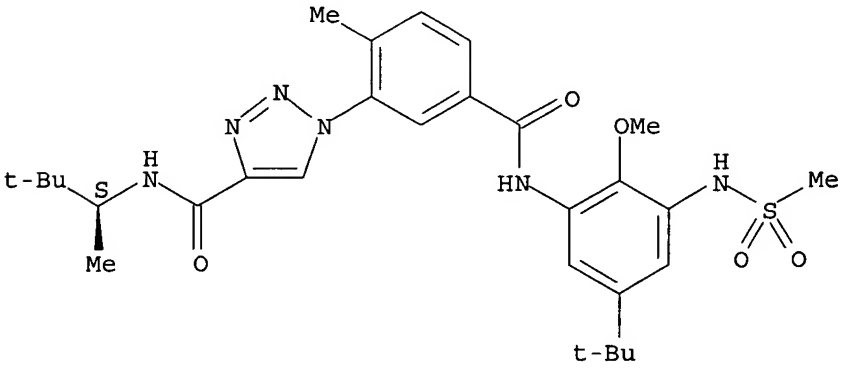


RN 695178-99-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-3-fluoro-2-methylphenyl]- (9CI) (CA INDEX NAME)

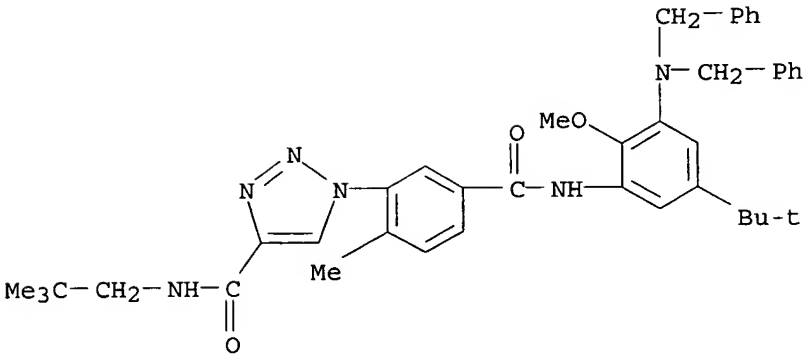


RN 695179-02-3 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[(1S)-1,2,2-trimethylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 695179-03-4 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[3-[bis(phenylmethyl)amino]-5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]-N-(2,2-dimethylpropyl)- (9CI) (CA INDEX NAME)



RN 695179-04-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-[1-(3-pyridinyl)ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 695178-24-6
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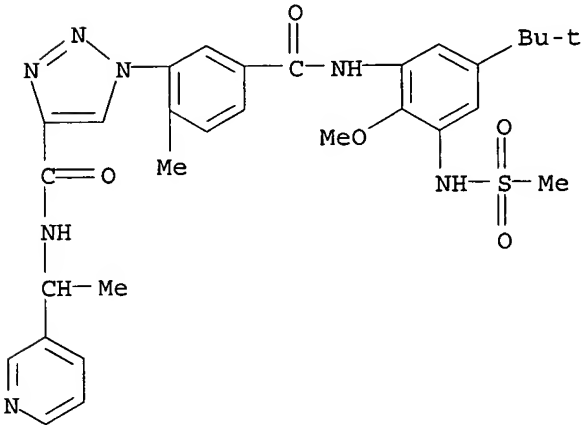
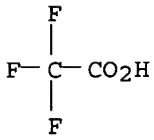


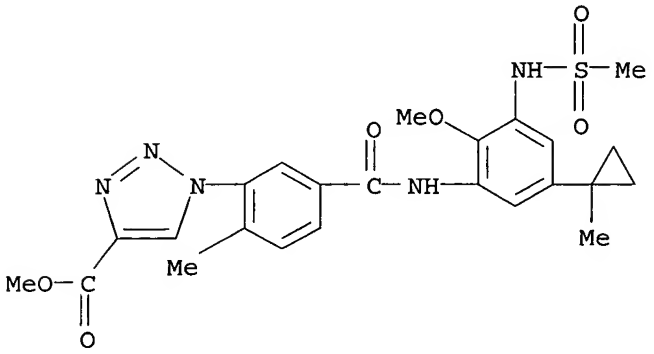
CM 2

CRN 76-05-1
CMF C2 H F3 O2

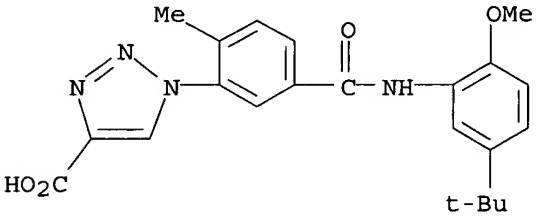


IT **702696-67-1 702699-41-0 702699-83-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aryltriazolecarboxylates as cytokine inhibitors)

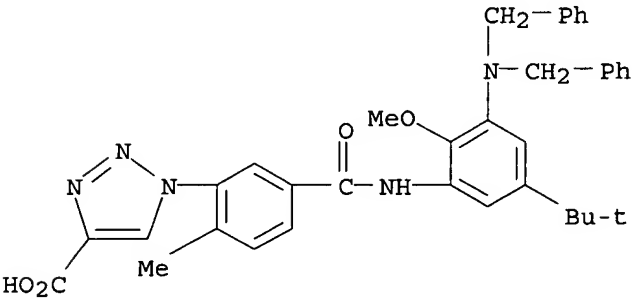
RN 702696-67-1 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[2-methoxy-5-(1-methylcyclopropyl)-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 702699-41-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

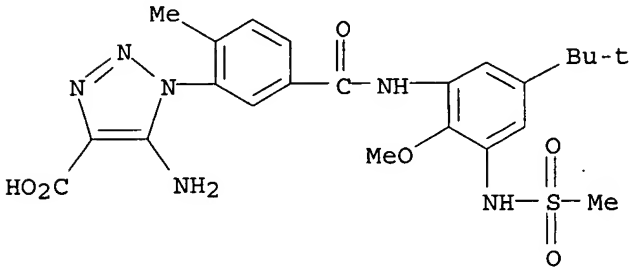


RN 702699-83-0 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[3-[bis(phenylmethyl)amino]-5-(1,1-dimethylethyl)-2-methoxyphenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

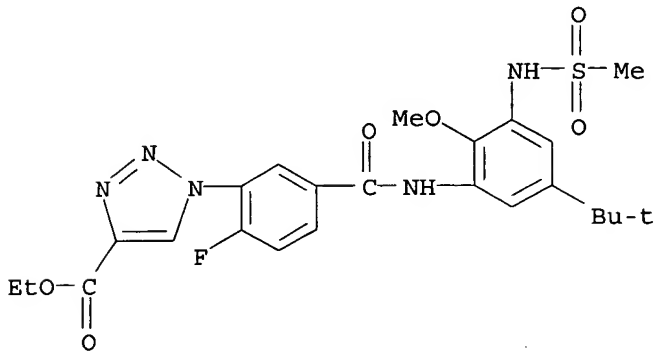


IT **695179-00-1P 695179-01-2P 695179-05-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryltriazolecarboxylates as cytokine inhibitors)
RN 695179-00-1 HCAPLUS

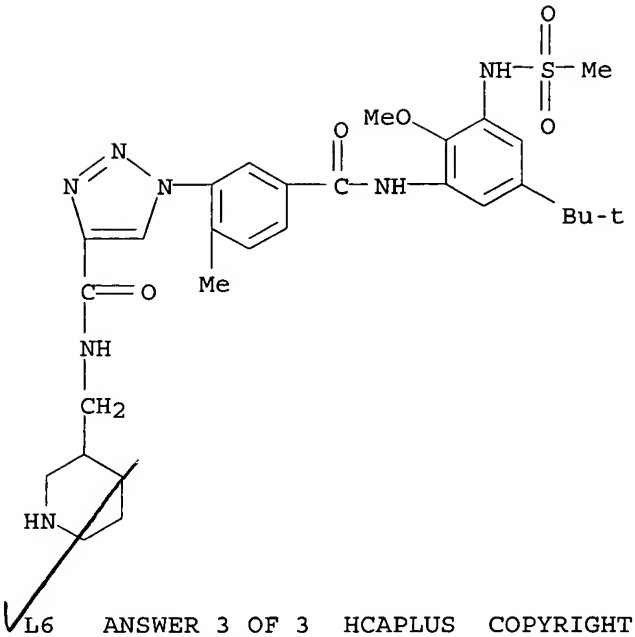
CN 1H-1,2,3-Triazole-4-carboxylic acid, 5-amino-1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)



RN 695179-01-2 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-fluorophenyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 695179-05-6 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxamide, 1-[5-[[[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]amino]carbonyl]-2-methylphenyl]-N-(3-piperidinylmethyl)- (9CI) (CA INDEX NAME)



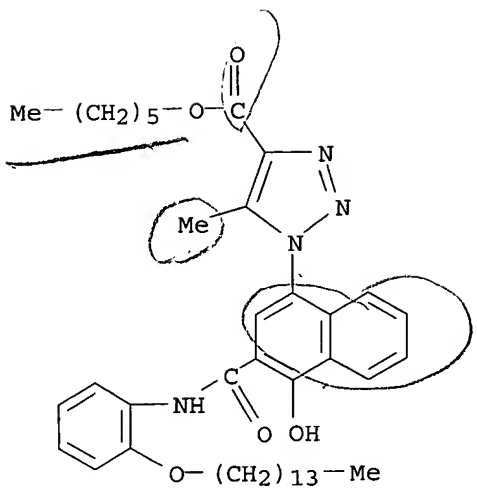
L6 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:540753 HCAPLUS
DOCUMENT NUMBER: 125:250364
TITLE: A new method for the synthesis of two-equivalent couplers in color photography
AUTHOR(S): Bergthaller, Peter
CORPORATE SOURCE: "Agfa-Gevaert" A.-G., Leverkusen, D-51301, Germany
SOURCE: Sulfur Reports (1996), 18(2), 337-359
CODEN: SUREDW; ISSN: 0196-1772
PUBLISHER: Harwood
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 29 refs. and new data of sulfanes preparation from photog. color couplers of the 1-naphthol, pyrazolo[5,1-c](1,2,4)triazole, and 3-anilinopyrazol-5-one classes. The sulfanes were transformed into hetero-substituted transient sulfur(IV) species capable of arylating a triazolate or carboxylate ligand or an added 1H-triazole via ligand exchange and a subsequent process closely related to ligand coupling. This new reaction is named sulfurane contraction and there is evidence for thiophilic control of the key steps involved. The syntheses are carried out preferably at ≈0° and provide access to photog. two-equivalent color couplers which are inaccessible by known methods.

IT **182292-73-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of two-equivalent couplers in color photog.)

RN 182292-73-5 HCAPLUS
CN 1H-1,2,3-Triazole-4-carboxylic acid, 1-[4-hydroxy-3-[[[2-(tetradecyloxy)phenyl]amino]carbonyl]-1-naphthalenyl]-5-methyl-, hexyl ester (9CI) (CA INDEX NAME)



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L9           17 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "QIAN K"/AU OR "QIAN K C"/AU
               OR ("QIAN KEVIN"/AU OR "QIAN KEVIN C"/AU OR "QIAN KEVIN
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L10          32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L7 OR L9) NOT L6


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L10  ANSWER 1 OF 32  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:1223820  HCAPLUS
DOCUMENT NUMBER:          143:460158
TITLE:                    Phenylpyrazoles and -imidazoles as anti-cytokines,
                          their preparation, pharmaceutical compositions, and
                          use in the treatment of inflammation and related
                          conditions
INVENTOR(S):              Cogan, Derek; Hao, Ming-Hong; Swinamer, Alan
                          David; Aungst, Ronald A.
PATENT ASSIGNEE(S):       Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE:                   U.S. Pat. Appl. Publ., 37 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     US 2005256113         A1    20051117    US 2005-120735          20050503
     WO 2005115991         A1    20051208    WO 2005-US15601         20050505
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
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RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2004-570284P P 20040512
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to compds. of formula I, which inhibit production of cytokines involved in inflammatory processes and are thus useful for treating diseases and pathol. conditions involving inflammation such as chronic inflammatory disease. In compds. I, Ar is selected from (un)substituted carbocyclyl, (un)substituted pyridinyl, and (un)substituted benzo ring fused to a 5- to 7-membered heterocyclic ring; R1 is OH, SH, NH2, alkoxy, alkylthio, (di)alkylamino, aryl, heteroaryl, heterocyclyl, etc.; R2 and R3 are independently selected from H, halo, C1-5 alkyl, C1-5 alkoxy, C1-5 alkyl-C1-5 alkoxy, OH, hydroxy-C1-5 alkyl, and amino, optionally mono- or di-substituted by C1-5 alkyl, aryl, or aryl-C1-5 alkyl; and V, W, X, and Y are independently selected from N and (un)substituted C, with 2 or 3 of those being N. The invention also relates to the preparation of I, pharmaceutical compns. containing a pharmaceutically effective amount of a compound I and one or more pharmaceutically acceptable carrier and/or adjuvants, as well as to the use of the compns. in the treatment of conditions involving inflammation. Diazotization of 3-amino-4-methylbenzoic acid followed by tin-mediated reduction gave the corresponding hydrazine, which underwent cyclocondensation with Et 2-formyl-3-oxopropionate to give pyrazole II. Compound II was coupled with N-(3-amino-5-tert-butyl-2-methoxyphenyl)-methanesulfonamide followed by ester hydrolysis and amidation with 3-(aminomethyl)pyridine, resulting in the formation of pyrazolecarboxamide III. The compds. of the invention block inflammatory cytokine production from cells (no data), with preferred compds. expressing IC50 values of less than 1 μM in an assay for inhibition of TNF production

L10 ANSWER 2 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1177572 HCAPLUS
DOCUMENT NUMBER: 143:422251
TITLE: Preparation of heterocyclic amides as cytokine inhibitors for treating various diseases
INVENTOR(S): Hao, Ming-Hong; Xiong, Zhaoming; Aungst, Ronald A.; Davis, Amy L.; **Cogan, Derek**; Goldberg, Daniel R.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 39 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2005245536 A1 20051103 US 2005-119524 20050429
WO 2005108387 A2 20051117 WO 2005-US14947 20050429
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2004-567693P P 20040503
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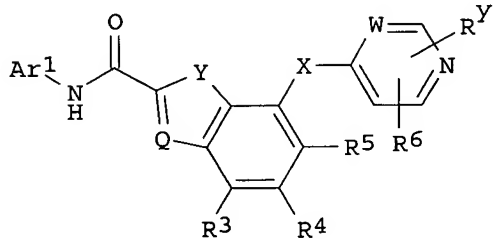

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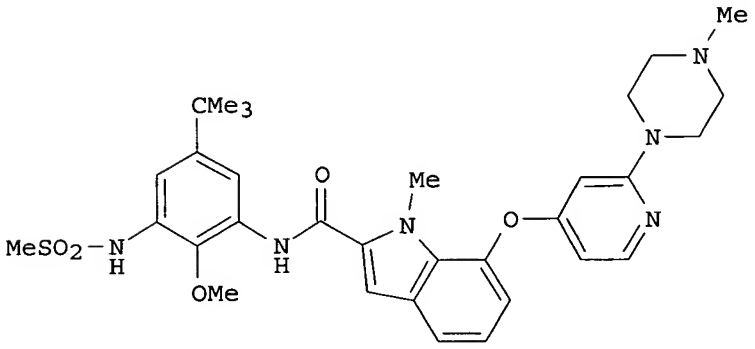

II

AB Disclosed are compds. of formula I (variables defined below) and pharmaceutically acceptable salts or isomers thereof that inhibit production of cytokines involved in inflammatory processes and are thus useful for treating diseases and pathol. conditions involving inflammation such as chronic inflammatory disease (no biol. data given). For I Ar = (un)substituted aryl, heterocycle, heteroaryl, or fused heterocycle; Q = N, (un)substituted CH; W = N, CH; X = CH2, O, S, (un)substituted NH; Y = O, S(O)m, (un)substituted CH2, CH=CH, NH; R3-R5 = independently H, halo, alkyl; R6 = a bond, O, O(CH2)1-5, CO, NH, CONH, S, (un)substituted alkyl, alkenyl, acyl, heterocyclyl, aryl; Ry = H or C1-5alkyl, m = 0-2. For example, a 9-step synthesis involving 3-methyl-2-nitrophenol, di-Et oxalate, 5-tert-butyl-3-methanesulfonamido-2-methoxyaniline, 2-chloro-4-iodopyridine, and 1-methylpiperazine as initial reactants gave II. Also disclosed are processes for preparing these compds. and pharmaceutical compns. comprising these compds.

L10 ANSWER 3 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1042236 HCAPLUS

DOCUMENT NUMBER: 143:347181
TITLE: Preparation of triazolyl arylbenzamides as inhibitors of cytokines
INVENTOR(S): **Cogan, Derek**; Hao, Ming-Hong; Kamhi, Victor Marc; Miller, Craig Andrew; Netherton, Matthew Russell; Swinamer, Alan David
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 226 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090333	A1	20050929	WO 2005-US6997	20050304

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PRIORITY APPLN. INFO.: US 2004-551445P P 20040309
OTHER SOURCE(S): MARPAT 143:347181
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Ar1 = substituted carbocycle, heteroaryl or benzofused heterocyclic ring; D, A, and B independently = H or CH wherein the hydrogen atom is optionally displaced by R3; Het = (un)substituted heterocycle or heteroaryl; R1, R2 and R3 independently = H, halo, OH, etc.; X = O or S] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of cytokines. Thus, e.g., II was prepared by cyclization of 2-chloro-5-ethynylpyridine (preparation given) with 3-azido-4-Me benzoic acid followed by coupling with N-(3-amino-5-tert-butyl-2-methoxy-phenyl)-methane-sulfonamide. The activity of I was evaluated by measuring the inhibition of TNFα in liposaccharide stimulated THP cells and preferred compds. have an IC50 below 1 μM in this assay (no data). I as inhibitors of cytokines should prove useful in the treatment of diseases such as but not limited to osteoarthritis, atherosclerosis and contact dermatitis. Pharmaceutical compns. comprising I are disclosed.
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

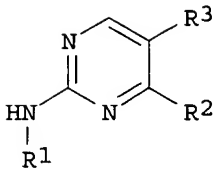
L10 ANSWER 4 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:634809 HCAPLUS
DOCUMENT NUMBER: 143:261009
TITLE: A hypoxia-inducible vigilant vector system for activating therapeutic genes in ischemia
AUTHOR(S): Tang, Y. L.; Tang, Y.; Zhang, Y. C.; Agarwal, A.;

Kasahara, H.; **Qian, K.**; Shen, L.; Phillips, M. I.
CORPORATE SOURCE: Department of Pediatrics, College of Medicine and All Children's Hospital Research Institute, University of South Florida, St Petersburg, FL, 33701, USA
SOURCE: Gene Therapy (2005), 12(15), 1163-1170
CODEN: GETHEC; ISSN: 0969-7128
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hypoxia represents an endogenous pathophysiol. signal underlying cell growth, adaptation and death in a variety of diseases, including ischemic heart diseases, stroke and solid tumors. A vigilant vector system depends on a gene switch which can sense the hypoxia signal occurring in ischemic events and turn on/off protective gene expressions when necessary. This system uses the oxygen-dependent degradation domain derived from hypoxia-inducible factor 1α as the hypoxia sensor and a double-vector system as signal amplifier. For treating ischemic heart diseases, a cardiac-specific MLC-2v promoter is used to deliver transgenes specifically to the heart. When tested in cardiomyocyte cultures, it produced a rapid and robust gene induction upon exposure to low oxygen. In a mouse model for myocardial infarction, the vigilant vectors turned on therapeutic genes such as heme oxygenase-1 in response to ischemia, significantly reduced apoptosis in the infarct area and improved cardiac functions. The hypoxia-regulated gene transfer afforded by the vigilant vectors may provide a powerful tool for delivering therapeutic proteins specifically to ischemic tissues with optimal physiol. control.
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:497492 HCAPLUS
DOCUMENT NUMBER: 143:7727
TITLE: Preparation of 2,4-diaminopyrimidine derivatives as inhibitors of PKC-theta for treating diseases associated with T cells activation, in particular immunol. disorders and type II diabetes
INVENTOR(S): Cardozo, Mario G.; **Cogan, Derek**; Cywin, Charles Lawrence; Dahmann, George; Disalvo, Darren; Ginn, John David; Prokopowicz, Anthony S.; Spero, Denice M.; Young, Erick Richard Roush
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.
SOURCE: U.S. Pat. Appl. Publ., 69 pp., Cont.-in-part of U.S. Ser. No. 766,079.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2005124640	A1	20050609	US 2004-933635		20040903
US 2004242613	A1	20041202	US 2004-766079		20040127
PRIORITY APPLN. INFO.:			US 2003-443700P	P	20030130
			US 2004-766079	A2	20040127

OTHER SOURCE(S): MARPAT 143:7727
GI



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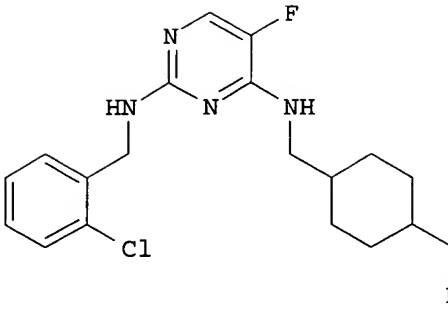
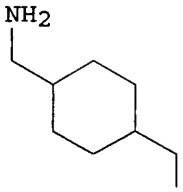


II



III

AB Title compds. I [wherein R1 = (un)substituted heteroaryl/aryl/cyclo/cycloalkyl/alkyl, naphthyl, quinolinyl, etc.; R2 = (un)substituted -NH-CH2-(CH2)n-CH2-NR4R5, -NH-(CH2)p-phenylene-(CH2)q-NR4R5, -NH(CH2)p-X-R4, etc.; X = piperidinyl; n = 3-8; p = 1-3; q = 0-3; R4, R5 = independently H, amidino, (un)substituted aryl/alkyl; R3 = halo, CN, NO2, aminocarbonyl, (un)substituted alkyl, alkyloxycarbonyl; their tautomers, pharmaceutically acceptable salts, solvates, or amino-protected derivs., with certain compds. excluded] were prepared as inhibitors of protein kinase C (PKC)-theta useful for treating immunol. disorders and type II diabetes. For example, II was prepared in 5 steps via amination of 2,4-dichloro-5-fluoropyrimidine with amine III and 2-chlorobenzylamine. Selected I inhibited PKC-theta with IC50 values ≤ 0.3 μM. Thus, I are useful for treating a disease or disorder associated with T cells activation.

L10 ANSWER 6 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:424368 HCAPLUS
DOCUMENT NUMBER: 143:42626
TITLE: The genetics characteristics of HLA alleles and haplotypes in the Shanghai han population
AUTHOR(S): Feng, M. L.; Xie, J. H.; Lu, Q.; Ji, Y.; Guo, X. J.; Yang, J. H.; Sun, J. L.; Liu, D. Z.; **Qian, K. C.**
CORPORATE SOURCE: Shanghai Institute of Blood Transfusion, Shanghai Blood Center, Shanghai, 200051, Peop. Rep. China
SOURCE: Current Genomics (2005), 6(2), 109-114
CODEN: CGUEA8; ISSN: 1389-2029
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Multilocus HLA haplotypes could be investigated by family anal., and there are salient differences in the distributions of HLA alleles among different populations. In the present study, HLA -A, B and DRB1 alleles and haplotypes were investigated based on 166 families in Shanghai Han

population by mol. biol. HLA typing methods and the distribution characteristic of HLA alleles and haplotypes were analyzed. The results of the authors' investigation showed that allele frequencies of more than 10% for HLA alleles were A*0201/07, A*1101, A*2402, B*4001, B*4601, DRB1*090102, DRB1*1202 and DRB1*15. In the anal. of HLA haplotypes, the authors identified 185 kinds of A-B haplotypes, 241 kinds of B-DRB1 haplotypes and 164 kinds of A-DRB1 haplotypes. Fifteen kinds of A-B haplotypes and 15 kinds of B-DRB1 haplotypes and 7 kinds of A-DRB1 haplotypes occurred at frequencies of more than 0.5% (linkage disequil. value $\Delta > 0$, $\chi 2 > 6.63$). Three hundred eighty-three kinds of A-B-DRB1 haplotypes were found and 20 kinds of A-B-DRB1 haplotypes occurred at frequencies of more than 0.5% ($\Delta > 0$). The common A-B-DRB1 haplotypes were A*3001-B*1302-DRB1*0701 (4.2%), A*0201/07-B*4601-DRB1*090102 (3.0%), A*3303-B*5801-DRB1*0301 (2.7%), A*3303-B*5801-DRB1*1301/02 (1.8%), A*1101-B*1502-DRB1*1202 (1.5%) and A*1101-B*3901-DRB1*0803 (1.1%). Comparison of the distribution of A-B-DRB haplotype among different populations revealed that Shanghai Han population has its own genetic characteristics, but are closed to East Asian populations and show more abundant polymorphism in the distribution of HLA alleles compare to East Asian populations. The result obtained in this study will be useful to provide information and instruction on Shanghai Han population for genetics, anthropol., association in diseases and forensic paternity testing. Equally encouraging is the potential benefit in helping patients search out healthy, matching hematopoietic stem cells.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:134678 HCAPLUS

DOCUMENT NUMBER: 142:369800

TITLE: Structural Basis of Constitutive Activity and a Unique Nucleotide Binding Mode of Human Pim-1 Kinase

AUTHOR(S): **Qian, Kevin C.**; Wang, Lian; Hickey, Eugene R.; Studts, Joey; Barringer, Kevin; Peng, Charline; Kronkaitis, Anthony; Li, Jun; White, Andre; Mische, Sheenah; Farmer, Bennett

CORPORATE SOURCE: Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Inc., Research and Development, Ridgefield, CT, 06877, USA

SOURCE: Journal of Biological Chemistry (2005), 280(7), 6130-6137
CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Pim-1 kinase is a member of a distinct class of serine/threonine kinases consisting of Pim-1, Pim-2, and Pim-3. Pim kinases are highly homologous to one another and share a unique consensus hinge region sequence, ER-PXPX, with its two proline residues separated by a non-conserved residue, but they (Pim kinases) have <30% sequence identity with other kinases. Pim-1 has been implicated in both cytokine-induced signal transduction and the development of lymphoid malignancies. We have determined the crystal structures of apo Pim-1 kinase and its AMP-PNP (5'-adenylyl-β,γ-imidodiphosphate) complex to 2.1-Å resolns. The structures reveal the following. (1) The kinase adopts a constitutively active conformation, and extensive hydrophobic and hydrogen bond interactions between the activation loop and the catalytic loop might be the structural basis for maintaining such a conformation. (2) The hinge region has a novel architecture and hydrogen-bonding pattern, which not only expand the ATP

pocket but also serve to establish unambiguously the alignment of the Pim-1 hinge region with that of other kinases. (3) The binding mode of AMP-PNP to Pim-1 kinase is unique and does not involve a critical hinge region hydrogen bond interaction. Anal. of the reported Pim-1 kinase-domain structures leads to a hypothesis as to how Pim kinase activity might be regulated in vivo.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:18540 HCAPLUS
DOCUMENT NUMBER: 142:331790
TITLE: Expression, purification, crystallization and preliminary crystallographic analysis of human Pim-1 kinase
AUTHOR(S): **Qian, Kevin C.**; Studts, Joey; Wang, Lian; Barringer, Kevin; Kronkaitis, Anthony; Peng, Charline; Baptiste, Alistair; LaFrance, Roger; Mische, Sheenah; Farmer, Bennett
CORPORATE SOURCE: Department of Medicinal Chemistry, Research and Development, Boehringer Ingelheim Pharmaceuticals Inc., Ridgefield, CT, 06877, USA
SOURCE: Acta Crystallographica, Section F: Structural Biology and Crystallization Communications (2005), F61(1), 96-99
CODEN: ACSFCL; ISSN: 1744-3091
URL: http://journals.iucr.org/f/issues/2005/01/00/en5073/index.html
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB Pim kinases, including Pim-1, Pim-2, and Pim-3, belong to a distinctive serine/threonine protein kinase family. They are involved in cytokine-induced signal transduction and the development of lymphoid malignancies. Their kinase domains are highly homologous to one another, but share low sequence identity to other kinases. Specifically, there are 2 Pro residues in the conserved hinge-region sequence ERPXPX separated by a residue that is non-conserved among Pim kinases. Here, full-length human Pim-1 kinase (1-313) was cloned and expressed in Escherichia coli as a GST-fusion protein and truncated to Pim-1 (14-313) by thrombin digestion during purification The Pim-1 (14-313) protein was purified to high homogeneity and monodispersity. This protein preparation yielded small crystals in the initial screening and large crystals after optimization. The large crystals of apo Pim-1 kinase diffracted to 2.1 Å resolution and belonged to space group P65, with unit-cell parameters a = b = 95.9, c = 80.0 Å, β = 120° and one mol. per asym. unit.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

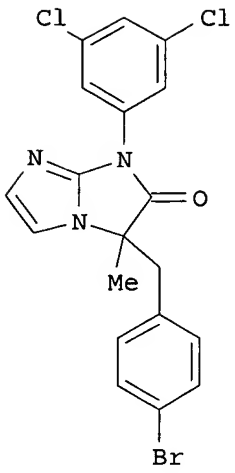
L10 ANSWER 9 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:791718 HCAPLUS
DOCUMENT NUMBER: 142:152479
TITLE: Study on the haplotypes of MICA and MICB microsatellite and HLA-B locus in the Guangzhou Han population
AUTHOR(S): Feng, M.-L.; Guo, X.-J.; Zhang, J.-Y.; Xie, J.-H.; Chen, L.; Lu, Q.; Yang, J.-H.; Ji, Y.; **Qian, K.-C.**
CORPORATE SOURCE: Shanghai Blood Center, Shanghai Institute of Blood Transfusion, Shanghai, Peop. Rep. China

SOURCE: Tissue Antigens (2004), 64(3), 281-285
CODEN: TSANA2; ISSN: 0001-2815
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The purpose of this study was to investigate the genetic polymorphisms and haplotypes of microsatellite locus to exon 5 of the MICA gene and intron 1 of the MICB gene and human leukocyte antigen-B (HLA-B) gene based on 106 samples of the Guangzhou Han population through means of polymerase chain reaction and the fluorescent technique (6-FAM). The corresponding haplotype frequencies, linkage disequil. values and relative linkage disequil. values were estimated based on population data. The results show that the genotype distributions of MICA and MICB microsatellite and HLA-B satisfy the Hardy-Weinberg equilibrium In total, five alleles of MICA microsatellite locus and 14 alleles of MICB microsatellite locus were observed MICA A5 was the most common allele (0.2877), whereas A4 was the least common (0.1321). MICB CA14 was the most common allele (0.3255), and CA19 and CA28 were the two least common (0.0047). CA27 was not observed at all. Five kinds of MICA-MICB haplotypes,18 kinds of MICA-HLA-B haplotypes and 12 kinds of MICB-HLA-B haplotypes occurred at frequencies of more than 1%. The common haplotypes of MICA-MICB, MICA-HLA-B and MICB-HLA-B were A5-CA14, A5.1-CA18, A4-CA26, A9-CA15, A5-B*15(62), A51-B*1301/1302, A4-B*1301/1302, A6-B*51, A6-B*4403, A9-B*3802, CA14-B*4601, CA18-B*1301/1302 and CA26-B*1301/1302, and these haplotypes showed strong linkage disequil. The polymorphisms and haplotype distributions of MICA and MICB microsatellite and HLA-B locus in the Guangzhou Han population have their own distinct genetic characteristics. The microsatellite locus of exon 5 of the MICA gene and intron 1 of the MICB gene could therefore be used as genetic markers in the studies of anthropol., gene linkage anal. in genetic diseases, individual identification and paternity testing in forensic medicine.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 10 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:790832 HCAPLUS
DOCUMENT NUMBER: 142:6469
TITLE: Second-generation lymphocyte function-associated antigen-1 inhibitors: 1H-imidazo[1,2-α]imidazol-2-one derivatives
AUTHOR(S): Emeigh, Jonathan; Gao, Donghong A.; Goldberg, Daniel R.; Kuzmich, Daniel; Miao, Clara; Potocki, Ian; **Qian, Kevin C.**; Sorcek, Ronald J.; Jeanfavre, Deborah D.; Kishimoto, Kei; Mainolfi, Elizabeth A.; Nabozny, Gerald, Jr.; Reilly, Patricia; Rothlein, Robert; Sellati, Rosemarie H.; Woska, Joseph R., Jr.; Chen, Shirlynn; Gunn, Jocelyn A.; O'Brien, Drane; Norris, Stephen H.; Kelly, Terence A.; Peng, Charline; Wu, Jiang-Ping
CORPORATE SOURCE: Research and Development, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(22), 5356-5366
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:6469
GI



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AB A novel class of lymphocyte function-associated antigen-1 (LFA-1) inhibitors is described. Discovered during the process to improve the physicochem. and metabolic properties of BIRT377, a previously reported hydantoin-based LFA-1 inhibitor, these compds. are 5- or 6-substituted derivs. of the 1H-imidazo[1,2-α]imidazol-2-one I. The structure-activity relationship (SAR) shows that electron-withdrawing groups at C(5) on the imidazole ring benefit potency and that oxygen-containing functional groups attached to a C(5)-sulfonyl or sulfonamide group further improve potency. This latter gain in potency is attributed to the interaction(s) of the functionalized sulfonyl/sulfonamide groups with the protein, likely polar-polar in nature, as suggested by SAR data. X-ray studies revealed that these bicyclic inhibitors bind to the I-domain of LFA-1 in a pattern similar to that of BIRT377.

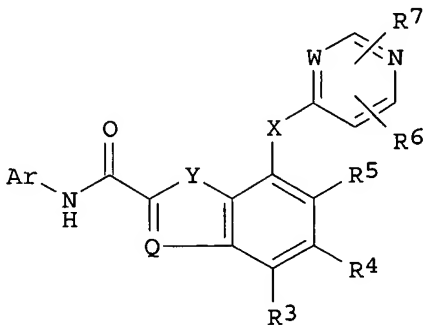
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:780360 HCAPLUS
DOCUMENT NUMBER: 141:295859
TITLE: Preparation of N-aryl-1H-indole-2-carboxamides as cytokine inhibitors
INVENTOR(S): Cirillo, Pier Francesco; Gao, Donghong Amy; Goldberg, Daniel R.; Hammach, Abdelhakim; Hao, Ming-Hong; Kamhi, Victor Marc; Moss, Neil; Netherton, Matthew Russell; **Qian, Kevin Chungeng**; Ralph, Mark Stephen; Wu, Lifen; Xiong, Zhaoming
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 82 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004186114	A1	20040923	US 2004-789354	20040227

CA 2518774 AA 20050224 CA 2004-2518774 20040302
WO 2005016918 A2 20050224 WO 2004-US6264 20040302
WO 2005016918 A3 20050407
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 2003-453364P P 20030310
WO 2004-US6264 W 20040302
OTHER SOURCE(S): MARPAT 141:295859
GI



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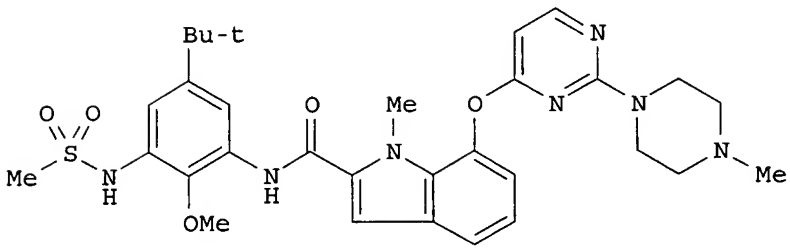

II

AB Title compds. I [wherein Ar = (un)substituted aryl; Q = N, (un)substituted CH; W = N, CH; X = CH2, O, S, (un)substituted NH; Y = O, SO0-2, (un)substituted CH2, CH=CH, NH; R3-R5 = independently H, halo, alkyl; R6 = a bond, O, O(CH2)1-5, CO, NH, CONH, S, (un)substituted alkyl, alkenyl, acyl, heterocyclyl, aryl; R7 = H, alkyl; and pharmaceutically acceptable salts, acids, or isomers thereof] were prepared For example, a 9-step synthesis starting from 3-methyl-2-nitrophenol, di-Et oxalate, 5-tert-butyl-3-methanesulfonamido-2-methoxyaniline, 2,4-dichloropyrimidine, and 1-methylpiperazine gave II. I inhibit production of cytokines involved in inflammatory processes and are, thus, useful for treating diseases and pathol. conditions involving inflammation, such as chronic inflammatory disease (no data). The compds. are also useful for treating diseases or conditions related to oncol. and anticoagulant or

fibrinolytic therapy (no data). Also disclosed are processes for preparing these compds. and pharmaceutical compns. comprising them.

L10 ANSWER 12 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:658082 HCAPLUS
TITLE: Discovery and design of novel benzimidazolone as inhibitors of p38 MAP kinase
AUTHOR(S): Hammach, Abdelhakim; Ralph, Mark; Corbo, Faith; Barbosa, Antonio; Liu, Pinrong; Soleymanzadeh, Fariba; Goldberg, Daniel; Sarko, Christopher; Mckibben, Brian; Moss, Neil; Hao, Ming-Hong; White, Andre; **Qian, Kevin**; Pargellis, Chris; Kroe, Rachel; Wildeson, Jessi; Nelson, Richard; Fadra, Tazmeen; Capolino, Alison; Kashem, Mohammed; Patnaude, Lori; Madwed, Jeff; Torcellini, Carol; Kaplita, Paul; Farrel, Tom; Hu, Hanbo; Yazdania, Mehran; Kavanaugh, Kelli
CORPORATE SOURCE: Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals Inc, Ridegefield, CT, 06877, USA
SOURCE: Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United States, August 22-26, 2004 (2004), MEDI-218. American Chemical Society: Washington, D. C.
CODEN: 69FTZ8
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB P38 Mitogen activated protein (MAP) kinase, a member of a group of serine-threonine kinases, has been shown to regulate the production of the pro-inflammatory cytokines TNF-alpha and IL-1. Inhibition of p38 is anticipated to have important therapeutic potential in inflammatory diseases such as rheumatoid arthritis, Crohn's disease and psoriasis. We utilized crystallog. information, mol. modeling and rational drug design to convert a hit obtained from high throughput screening to mols. of general structure 1. This presentation will focus on the design process for achieving key interactions with the protein, key SAR observations as well as the synthetic strategy towards these p38 inhibitors.

L10 ANSWER 13 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:648512 HCAPLUS
DOCUMENT NUMBER: 141:190795
TITLE: Preparation of 2,4-diaminopyrimidine derivatives as inhibitors of PKC-theta for treating diseases associated with T cells activation, in particular immunol. disorders and type II diabetes
INVENTOR(S): Cardozo, Mario G.; **Cogan, Derek**; Cywin, Charles Lawrence; Dahmann, Georg; Disalvo, Darren; Ginn, John David; Prokopowicz, Anthony S.; Spero, Denice M.; Young, Erick Richard Roush
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA; Boehringer Ingelheim Pharma GmbH & Co. KG
SOURCE: PCT Int. Appl., 124 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067516	A1	20040812	WO 2004-US2240	20040127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,				

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI

CA 2514612	AA	20040812	CA 2004-2514612	20040127
EP 1590334	A1	20051102	EP 2004-705675	20040127

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:	US 2003-443700P	P	20030130
	WO 2004-US2240	W	20040127

OTHER SOURCE(S): MARPAT 141:190795
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = (un)substituted heteroaryl/aryl/cyclo/cycloalkyl/alkyl, naphthyl, quinolinyl, etc.; R2 = (un)substituted -NH-CH2-(CH2)n-CH2-NR4R5, -NH-(CH2)p-phenylene-(CH2)q-NR4R5, -NH(CH2)p-X-R4, etc.; X = pyridinyl; n = 3-8; p = 1-3; q = 0-3; R4, R5 = independently H, amidino, (un)substituted aryl/alkyl; R3 = halo, CN, NO2, aminocarbonyl, (un)substituted alkyl, alkyloxycarbonyl; their tautomers, pharmaceutically acceptable salts, solvates, or amino-protected derivs., with certain compds. excluded] were prepared as inhibitors of protein kinase C (PKC)-theta useful for treating immunol. disorders and type II diabetes. For example, II was prepared in 5 steps via amination of 2,4-dichloro-5-fluoropyrimidine with amine III and 2-chlorobenzylamine. Selected I inhibited PKC-theta with IC50 values ≤ 0.3 μM. Thus, I are useful for treating a disease or disorder associated with T cells activation.

L10 ANSWER 14 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2003:837072 HCAPLUS
DOCUMENT NUMBER:	139:337887
TITLE:	Preparation of heterocyclic amide derivatives as cytokine inhibitors
INVENTOR(S):	Gao, Donghong Amy; Goldberg, Daniel R.; Hammach, Abdelhakim; Hao, Ming-Hong; Moss, Neil; **Qian, Kevin Chungeng**; Roth, Gregory Paul; Sarko, Christopher Ronald; Swinamer, Alan David; Xiong, Zhaoming; Kamhi, Victor Marc
PATENT ASSIGNEE(S):	Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE:	PCT Int. Appl., 96 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003087085	A1	20031023	WO 2003-US11094	20030410

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2478232	AA	20031023	CA 2003-2478232		20030410
US 2003225053	A1	20031204	US 2003-410688		20030410
EP 1497278	A1	20050119	EP 2003-721619		20030410
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2005530730	T2	20051013	JP 2003-584041		20030410
PRIORITY APPLN. INFO.:			US 2002-371671P	P	20020411
			WO 2003-US11094	W	20030410

OTHER SOURCE(S): MARPAT 139:337887

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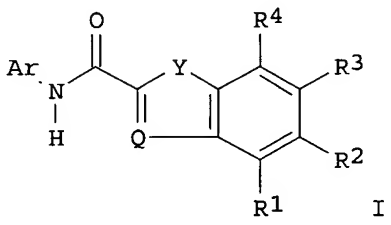

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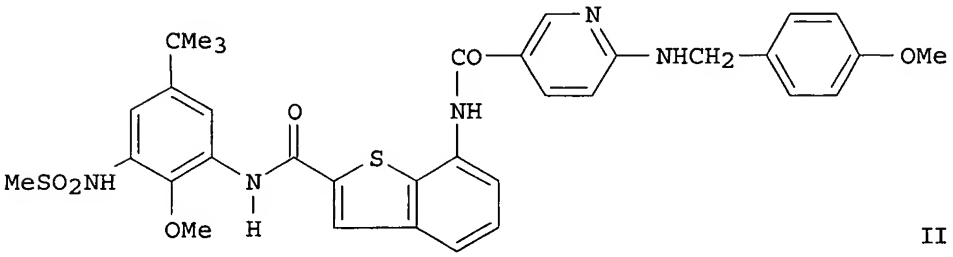

II

AB Amides I [Q = N, (un)substituted CH; Y = (un)substituted CH2, CH:CH, O, NH, S, S(O), SO2; Ar = (un)substituted carbocyclic; R1, R4 = H, halogen, OH, CN, (un)substituted alkyl, alkenyl, alkynyl, NH2, alkoxy, alkylthio, acyl, alkoxycarbonyl, acyloxy; R2, R3 = H, alkyl, halogen] were prepared as inhibitors of the production of cytokines involved in inflammatory processes and are thus useful for treating diseases and pathol. conditions involving inflammation such as chronic inflammatory disease (no data). Thus, the amide II was prepared from 2-chloro-3-nitrobenzoic acid in 8 steps.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:332822 HCAPLUS

TITLE: Asymmetric synthesis of amines and α,α-disubstituted amino acids from tert-butanesulfinyl ketimines.

AUTHOR(S): Borg, George; **Cogan, Derek A.**; Ellman, Jonathan A.

CORPORATE SOURCE: Chemistry, Ellman Research Group, U of CA, Berkeley, CA, 94596, USA

SOURCE: Book of Abstracts, 219th ACS National Meeting, San

Francisco, CA, March 26-30, 2000 (2000), ORGN-695. American Chemical Society: Washington, D. C.
CODEN: 69CLAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB A one-pot method for the asym. reductive amination of ketones with NaBH4 is described. Ketones 2 are condensed with (R)-tert-butanesulfinamide 1 to form tert-butanesulfinyl imine (R)-3, which are reduced in situ with NaBH4 to afford sulfinamides 4 in 66-86% yield and drs ranging from 90:10 to 97:3. In this procedure, Ti(OEt)4 serves as both a water scavenger and catalyst for imine condensation, and as a Lewis acid that provides enhanced reduction rates and drs. We have also applied tert-butanesulfinyl ketimines to the asym. synthesis of α ,α -disubstituted amino acids. Nucleophilic addns. of 2-methylfuryllithium to sulfinyl imines (R)-3 in the presence of AlMe3 afford sulfinamides 5 in 75-97% yield with drs ranging from 75:25 to 99:1. Subsequent oxidation with RuCl3-H2O and NaIO4 affords the tert-butanesulfonyl-protected α ,α -disubstituted amino acid 6 in 60% yield an acid/base extraction

L10 ANSWER 16 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:104443 HCAPLUS
DOCUMENT NUMBER: 133:43219
TITLE: The preparation of tert-butanesulfinamide and its application in the asymmetric synthesis of chiral amines
AUTHOR(S): **Cogan, Derek Alan**
CORPORATE SOURCE: Univ. of California, Berkeley, CA, USA
SOURCE: (1999) 153 pp. Avail.: UMI, Order No. DA9931215
From: Diss. Abstr. Int., B 1999, 60(6), 2695
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable

L10 ANSWER 17 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:569659 HCAPLUS
DOCUMENT NUMBER: 131:310266
TITLE: One-pot asymmetric synthesis of tert-butanesulfinyl-protected amines from ketones by the in situ reduction of tert-butanesulfinyl ketimines
AUTHOR(S): Borg, George; **Cogan, Derek A.**; Ellman, Jonathan A.
CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Tetrahedron Letters (1999), 40(37), 6709-6712
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:310266
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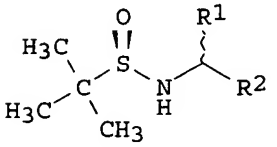


I

AB A one-pot method for the asym. synthesis of tert-butylsulfinyl-protected amines I (R1 = Me, Bu; R2 = Ph, i-Pr, Bu, i-Bu, PhCH2, 4-NCC6H4, (E)-CH:CHC6H4) is described. Ketones R1COR2 are condensed with (R)-tert-butanesulfinamide. The tert-butylsulfinyl imine intermediates (CH3)3CS(O)N:CR1R2 are then reduced in situ with NaBH4 to afford the sulfinamides (R,R)- and (R,S)-I in 66-86% yields and with diastereomeric ratios from 90:10 to 97:3 for both aryl alkyl and dialkyl ketones. Ti(OEt)4 serves as both a water scavenger and catalyst for imine condensation and as a Lewis acid that provides enhanced reduction rates and diastereomeric ratios.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:457654 HCAPLUS
DOCUMENT NUMBER: 131:242774
TITLE: Asymmetric synthesis of chiral amines by highly diastereoselective 1,2-additions of organometallic reagents to N-tert-butanesulfinyl imines
AUTHOR(S): **Cogan, Derek A.**; Liu, Guangcheng; Ellman, Jonathan
CORPORATE SOURCE: Department of Chemistry, University of California at Berkeley, Berkeley, CA, 94720, USA
SOURCE: Tetrahedron (1999), 55(29), 8883-8904
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:242774

AB High yielding and highly diastereoselective methods for 1,2-addns. of organometallic reagents to N-tert-butanesulfinyl aldimines and N-tert-butanesulfinyl ketimines were described. The addition of alkyl, aryl, alkenyl, and allyl carbanions to a diverse set of imines with different steric and electronic properties are demonstrated. Acidic methanolysis of the sulfinamide products delivers highly enantioenriched α-branched and α,α-branched amines. Since a broad range of sulfinyl imines are easily accessible from aldehydes and ketones, a wide variety of enantioenriched amines may be prepared For example, the addition of methylmagnesium bromide to [N(E),S(R)]-2-methyl-N-(2-methylpropylidene)-2-propanesulfinamide gave [S(R)]-2-methyl-N-[(S)-1,2-dimethylpropyl]--2-propanesulfinamide. After hydrolysis, the latter yielded (S)-3-methyl-2-butanamine hydrochloride.

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 19 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:76013 HCAPLUS
DOCUMENT NUMBER: 130:237100
TITLE: Synthesis of Enantiomerically Pure N-tert-Butanesulfinyl Imines (tert-Butanesulfinimines) by the Direct Condensation of tert-Butanesulfinamide with Aldehydes and Ketones
AUTHOR(S): Liu, Guangcheng; **Cogan, Derek A.**; Owens, Timothy D.; Tang, Tony P.; Ellman, Jonathan A.
CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Journal of Organic Chemistry (1999), 64(4), 1278-1284
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Exptl. details for the first general methods for the one-step preparation of N-tert-butanesulfinyl imines (tert-butanesulfinimines) from aldehydes and ketones is described. To effect the condensations of tert-butanesulfinamide with aldehydes, the Lewis acidic dehydrating agents MgSO4, CuSO4, or Ti(OEt)4 are employed. Aldehyde condensations mediated by MgSO4 proceed in high yields (84-96%) when an excess of aldehyde is used. In contrast, only a slight excess of aldehyde (1.1 equiv) relative to tert-butanesulfinamide provides sulfinimines in high yields when the more Lewis acidic dehydrating agent CuSO4 is used. The CuSO4-mediated procedure is effective for a wide range of aldehydes, including sterically demanding aldehydes, such as isobutyraldehyde (90%), and electron-rich aldehydes, such as p-anisaldehyde (81%). The still more Lewis acidic Ti(OEt)4 and Ti(O-i-Pr)4 also afford N-tert-butanesulfinyl aldimines from especially unreactive aldehydes, such as pivaldehyde (82%). In addition, Ti(OEt)4 is effective for the condensation of tert-butanesulfinamide with ketones to afford a wide range of N-tert-butanesulfinyl ketimines in good yields (77-91%). For sulfinyl ketimines derived from Me or n-alkyl Ph ketones and Me or n-alkyl iso-Pr ketones, only the E isomer is detected by 1H and 13C NMR in CDCl3. For those cases where the difference in steric demand about the imine is very small, such as for 2-hexanone, high E/Z ratios are still observed (5:1).

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 20 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:807964 HCAPLUS

DOCUMENT NUMBER: 130:130978

TITLE: Bubble coverage and bubble resistance using cells with horizontal electrode

AUTHOR(S): **Qian, K.**; Chen, Z. D.; Chen, J. J. J.

CORPORATE SOURCE: Department of Chemical & Materials Engineering, The University of Auckland, Auckland, 92019, N. Z.

SOURCE: Journal of Applied Electrochemistry (1998), 28(10), 1141-1145
CODEN: JAELBJ; ISSN: 0021-891X

PUBLISHER: Chapman & Hall

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The resistivity ratio due to gas bubbles underneath horizontal anodes in electrolytic cells was measured and compared with that in an air-water model of identical geometry. At equal c.d. or equivalent gas generation rate, the difference in the bubble resistivity ratio between these two situations can be up to 20%. Consequently, the results obtained from an air-water model cannot be directly applied to an electrolytic cell. Also within the range of exptl. conditions covered, the bubble resistivity ratios obtained for a given anode-cathode distance in both cells are linearly related to the bubble coverage ratio, based on bubbles greater than a certain size as limited by the measurement method.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 21 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:804828 HCAPLUS

DOCUMENT NUMBER: 130:153356

TITLE: Asymmetric Synthesis of α,α-Dibranched Amines by the Trimethylaluminum-Mediated 1,2-Addition of Organolithiums to tert-Butanesulfinyl Ketimines

AUTHOR(S): **Cogan, Derek A.**; Ellman, Jonathan A.

CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Journal of the American Chemical Society (1999), 121(1), 268-269
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:153356

AB Tert-alkyl benzylamides PhCONHCRR1R2 I [R = Me, Ph, Me(CH2)3; R1 = Me, Me2CH; R2 = Me2CH, Me(CH2)3, Me2CHCH2, Ph] are prepared in 61-100% yield and with diastereomer ratios from 91:9 to 99:1 by stereoselective nucleophilic addition of organolithium reagents RLi (R = Me, Bu, Ph) to tert-butylsulfinylimines (E, RS)-Me3CS(:O)N:CR1R2 II in the presence of 1.1 equivalent Me3Al followed by deprotection with HCl in methanol and benzoylation. II are prepd.in 66-88% yields by the direct condensation of (RS)-Me3CS(:O)NH2 with ketones in the presence of Ti(OEt)4, producing the (E)-sulfinylimines stereoselectively.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 22 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:530609 HCAPLUS
TITLE: The asymmetric synthesis of alpha,alpha-disubstituted amines via tert-butanesulfinimines derived from ketones.
AUTHOR(S): **Cogan, D. A.**; Liu, G.; Ellman, J. A.
CORPORATE SOURCE: Department Chemistry, University California, Berkeley, CA, 94720, USA
SOURCE: Book of Abstracts, 216th ACS National Meeting, Boston, August 23-27 (1998), ORGN-246. American Chemical Society: Washington, D. C.
CODEN: 66KYA2
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

AB We recently described a highly practical synthesis of tert-butanesulfinamide, 1, where the key step is the asym. oxidation of the inexpensive tert-Bu disulfide. We further described conditions for the condensation of 1 with aldehydes to provide sulfinimines, 2 (R1=H), and the addition of Grignard reagents into 2 in high yield and with excellent diastereoselectivity to provide the corresponding sulfinamides, 3. We will describe an important extension of this work, first with the condensation of 1 with ketones providing 2 (R1≠H) in high yields. The highly diastereoselective addition of common organometallic compds. into 2 will also be described. The alpha,alpha-disubstituted amines, 4, obtained after sulfinyl cleavage are unavailable by other methods. [Equation Omitted].

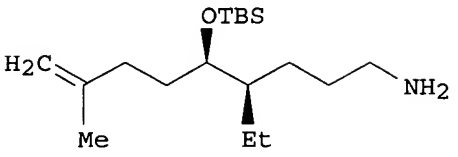
L10 ANSWER 23 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:499359 HCAPLUS
DOCUMENT NUMBER: 129:216215
TITLE: Catalytic Asymmetric Oxidation of tert-Butyl Disulfide. Synthesis of tert-Butanesulfinamides, tert-Butyl Sulfoxides, and tert-Butanesulfinimines
AUTHOR(S): **Cogan, Derek A.**; Liu, Guangcheng; Kim, Kyungjin; Backes, Bradley J.; Ellman, Jonathan A.
CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Journal of the American Chemical Society (1998), 120(32), 8011-8019

CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:216215
AB The first example of the catalytic asym. oxidation of tert-Bu disulfide (1) is described. The product, tert-Bu tert-butanethiosulfinate (2) is obtained with 91% enantiomeric excess in yields of ≥92% on scales as large as 1 mol. The application of H2O2 as stoichiometric oxidant in the presence of 0.25 mol % of VO(acac)2 and 0.26 mol % of a chiral Schiff base ligand is both convenient and cost-effective. Thiosulfinate ester 2 is chemical and optically stable and serves as an excellent precursor to chiral tert-butanesulfinyl compds. by the stereospecific nucleophilic displacement of tert-Bu thiolate. Addition of LiNH2 in liquid ammonia and THF provides tert-butanesulfinamide (91% yield). Enantiomerically pure thiosulfinate ester 2 also reacts readily and stereospecifically with Grignard reagents, organolithiums, lithium amides, and lithium imine salts to provide enantiomerically pure chiral sulfoxides, sulfinamides, and sulfinimines in good yield.
REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 24 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:141471 HCAPLUS
TITLE: Characterization and classification of gas oils by mass spectrometry for application in fluid catalytic cracking.
AUTHOR(S): **Qian, K.**; Peru, D. A.; Petti, T. F.; Zhao, X.; Yaluris, G.; Harding, R. H.; Cheng, W-C.; Rajagopalan, K.
CORPORATE SOURCE: Grace Davison, Columbia, MD, 21044, USA
SOURCE: Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2 (1998), PETR-089. American Chemical Society: Washington, D. C.
CODEN: 65QTAA
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Gas oils for fluid catalytic cracking (FCC) contain immense nos. of hydrocarbon compds. and isomers which directly impact FCC catalysts performance. There is a growing interest among refineries and catalyst manufacturers in developing correlations among feed composition and catalyst properties, in order to optimize FCC cracking conditions and catalyst selection strategies. We will discuss fundamentals of mol. characterization of gas oils, which has been a subject of extensive studies over the past four decades and a cornerstone for understanding the roles of feedstock components in the FCC process. We will also discuss combinations of mass spectrometry and chemometrics for rapid classification of gas oils based on their chemical composition These techniques allow us to evaluate feed selectivity in the FCC process and obtain more detailed understandings of feed/catalyst interactions.

L10 ANSWER 25 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:667400 HCAPLUS
DOCUMENT NUMBER: 127:346583
TITLE: Applications of Zr-Catalyzed Carbo-Magnesation and Mo-Catalyzed Macrocyclic Ring Closing Metathesis in Asymmetric Synthesis. Enantioselective Total Synthesis of Sch 38516 (Fluvirucin B1)
AUTHOR(S): Xu, Zhongmin; Johannes, Charles W.; Houri, Ahmad F.;

La, Daniel S.; **Cogan, Derek A.**; Hofilena, Gloria E.; Hoveyda, Amir H.
CORPORATE SOURCE: Department of Chemistry Merkert Chemistry Center, Boston College, Chestnut Hill, MA, 02167, USA
SOURCE: Journal of the American Chemical Society (1997), 119(43), 10302-10316
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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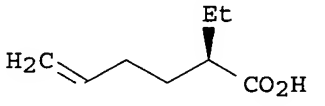

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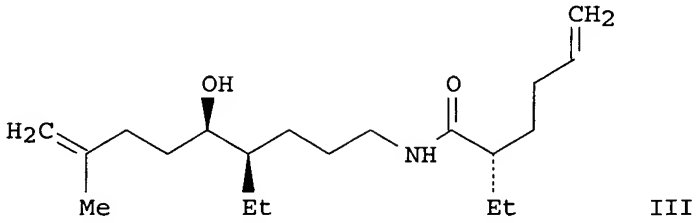

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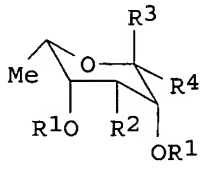

IV

AB The first enantioselective total synthesis of antifungal agent Sch 38516, also known as fluvirucin B1, is described. The synthesis includes a convergent asym. preparation of amine I and acid II, which are then united to afford diene III. Metal-catalyzed transformations play a crucial role in the synthesis of the latter moiety. Of particular note are the diastereo- and enantioselective Zr-catalyzed alkylations, a tandem Ti- and Ni-catalyzed process that constitutes a hydrovinylation reaction, and a Ru-catalyzed alc. oxidation to afford carboxylic acid II. The requisite carbohydrate IV (R1 = H; R2 = NH2.HCl; R3 = OH; R4 = H)is synthesized in a highly diastereo- and enantioselective fashion. Optical purity of the carbohydrate moiety arises from the use of the asym. dihydroxylation method of Sharpless; diastereochem. control is achieved through a selective dipolar [3 + 2] cycloaddn. with a readily available amine serving as the chiral auxiliary. Union of the appropriately outfitted carbohydrate IV (R1 = acetyl; R2 = NH-CO-CF3; R3,R4 = F, H) and diene III through an efficient and diastereoselective glycosidation is followed by a

remarkably efficient Mo-catalyzed macro-cyclization that proceeds readily at room temperature
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 26 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:667233 HCAPLUS
DOCUMENT NUMBER: 127:292929
TITLE: Catalytic Asymmetric Synthesis of tert-Butanesulfinamide. Application to the Asymmetric Synthesis of Amines
AUTHOR(S): Liu, Guangcheng; **Cogan, Derek A.**; Ellman, Jonathan A.
CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Journal of the American Chemical Society (1997), 119(41), 9913-9914
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:292929
AB An efficient two-step synthesis of optically pure tert-butanesulfinamide (R)-Me3CSONH2 in 75% overall yield from the inexpensive starting material tert-Bu disulfide, is reported. The key step is asym. catalytic oxidation of tert-Bu disulfide to provide tert-Bu tert-butanethiosulfinate using a vanadium catalyst, H2O2 as the stoichiometric oxidant, and a chiral ligand prepared by condensation of 3,5-di-tert-butylsalicylaldehyde and (S)-tert-leucinol. This reaction has been performed reproducibility on a half mol scale at 1.5 M concentration in CHCl3 with 1% catalyst to provide a 96-98% yield of pure product in 91% ee, after bulb to bulb distillation The utility of the tert-butanesulfinamide for the asym. synthesis of amines is also reported. Direct condensation of tert-butanesulfinamide with aldehydes provides the tert-butanesulfinimines in high yields (91-96%). Nucleophilic addns. proceed in high yield (>90%) for a range of Grignard reagents and sulfinimine substrates. The reaction diastereoselectivities are also high (89:11 to 98:2). Removal of the sulfinyl group to provide the scalemic amine hydrochlorides is accomplished by treatment of sulfinamides with HCl in methanol followed by ether precipitation (88-97% yields).
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 27 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:300074 HCAPLUS
DOCUMENT NUMBER: 127:72096
TITLE: Visual observation of bubbles at horizontal electrodes and resistance measurements on vertical electrodes
AUTHOR(S): **Qian, K.**; Chen, J. J. J.; Matheou, N.
CORPORATE SOURCE: Dep. of Chem. & Materials Eng., Univ. of Auckland, N. Z.
SOURCE: Journal of Applied Electrochemistry (1997), 27(4), 434-440
CODEN: JAELBJ; ISSN: 0021-891X
PUBLISHER: Chapman & Hall
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the Hall-Heroult process used in Al reduction cells, the electrodes are set in horizontal orientation and gas bubbles are generated on the underside of the anode which is immersed in the electrolyte. A comparison was made

of the bubbles formed on a horizontal bottom-facing electrode in a phys. analog model with those formed electrolytically. Bubbles formed in a phys. analog model by forcing air through a porous plate are larger, with wetted clear areas between bubbles. By contrast, electrolytically generated gas bubbles are smaller and the electrode surface is covered with a foamy layer of tiny bubbles. To measure the bubble resistance on horizontal electrodes, a method was developed for vertical electrodes so that the measurements may be validated by comparison with published data. Voltage fluctuations were measured and analyzed by using a fast Fourier transform (FFT). The magnitude of the bubble impedance was obtained at a superimposed a.c. frequency f0. The phase angle caused by the effects of the double layer capacitance and the faradaic impedance on bubble resistance was determined The effects of the faradaic impedance and the double layer capacitance were negligibly small under exptl. conditions.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 28 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:925144 HCAPLUS
TITLE: The fluid catalytic cracking selectivities of gas oil boiling point and hydrocarbon fractions
AUTHOR(S): Harding, R. H.; Zhao, X.; **Qian, K.**; Rajagopalan, K.; Cheng, W. C.; Davison, Grace
CORPORATE SOURCE: W.R. Grace and Co., CT, USA
SOURCE: Book of Abstracts, 210th ACS National Meeting, Chicago, IL, August 20-24 (1995), Issue Pt. 2, PETR-067. American Chemical Society: Washington, D. C.
CODEN: 61XGAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

AB The product selectivities of the Fluid Catalytic Cracking (FCC) process strongly dependent on the properties of the petroleum gas oil reactant. In order to elucidate the complex relationship between gas oil chemical composition and product selectivity, a new technique has been developed which exptl. dets. the product distribution of specific gas oil fractions in a realistic chemical environment. This "Incremental Yield Anal." approach is examined with a representative industrial gas oil. The gas oil is characterized and then divided into b.p. fractions by distillation and into hydrocarbon-type fractions with a chromatog. method. The FCC selectivity of each gas oil fraction is then determined by Microactivity testing of blends of each fraction with the original gas oil. Results show that hydrocarbon type is a more significant determinant of the product spectrum than b.p.

L10 ANSWER 29 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:413380 HCAPLUS
DOCUMENT NUMBER: 122:187230
TITLE: Cascade catalysis in synthesis. An enantioselective route to Sch 38516 (and fluvirucin B1) aglycon macrolactam
AUTHOR(S): Houri, Ahmad F.; Xu, Zhongmin; **Cogan, Derek A.**; Hoveyda, Amir H.
CORPORATE SOURCE: Merkert Chemistry Center, Boston College, Chestnut Hill, MA, 02167, USA
SOURCE: Journal of the American Chemical Society (1995), 117(10), 2943-4
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:187230
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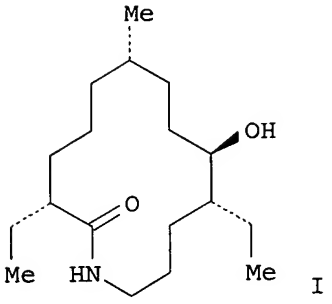

I

AB The Sch 38516 (fluvirucin B1) aglycon I has been synthesized efficiently and enantioselectively by a general scheme that can be easily modified for the preparation of the other members of this class of natural products. Importantly, all issues of carbon-carbon bond formation and stereochem. are addressed by metal-catalyzed processes. The Zr-catalyzed regio-, diastereo-, and enantioselective carbomagnesiations readily provide intermediates (5R,6R)-H2C:CMe(CH2)2CH(OH)CHEt(CH2)3NHTs (Ts = 4-MeC6H4SO2) and (S)-H2C:CHCHEtCH2OH. The synthesis scheme presented herein contains two critical steps where multiple operations are carried out in a single vessel, a strategy that is economically and environmentally attractive. These studies demonstrate that the Mo-catalyzed diene-metathesis can be used in the synthesis of macrocycles in the absence of a rigid mol. framework, providing a powerful route to the stereoselective formation of unsatd. large ring systems.

L10 ANSWER 30 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:210215 HCAPLUS
DOCUMENT NUMBER: 114:210215
TITLE: On-line liquid chromatography/mass spectrometry for heavy hydrocarbon characterization
AUTHOR(S): Hsu, Chang S.; McLean, M. A.; **Qian, K.**; Aczel, T.; Blum, S. C.; Olmstead, W. N.; Kaplan, L. H.; Robbins, W. K.; Schulz, W. W.
CORPORATE SOURCE: Exxon Res. and Eng. Co., Annandale, NJ, 08801, USA
SOURCE: Energy & Fuels (1991), 5(3), 395-8
CODEN: ENFUEM; ISSN: 0887-0624
DOCUMENT TYPE: Journal
LANGUAGE: English

AB There are many advantages of using online liquid chromatog./mass spectrometer (LC/MS) to characterize complex mixts. By incorporating low-voltage electron-impact ionization/high-resolution MS with moving belt LC/MS, differentiation can be made between naphthenoaroms. and alkylaroms. and between aromatic hydrocarbons and "difficult-to-resolve" thiophenes. Alternative online LC/MS techniques for heavy hydrocarbon characterization are also discussed.

L10 ANSWER 31 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:591111 HCAPLUS
DOCUMENT NUMBER: 113:191111
TITLE: Reactions of chloramine with methylpyridines. Synthesis and crystal structure of N-amino-3,5-dimethylpyridinium chloride

AUTHOR(S): Palenik, Gus J.; **Qian, K.**; Koziol, A. E.; Sisler, Harry H.
CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
SOURCE: Inorganic Chemistry (1990), 29(20), 4016-18
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:191111
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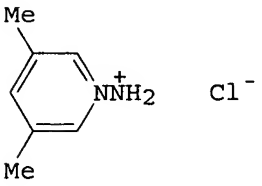

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AB The reactions of 2,4-, 2,3-, and 3,5-lutidine and 2,4,6-collidine with ether solns. of chloramine were examined Only in the case of 3,5-lutidine was an amination product obtained. In the other cases ammonium chloride and the hydrochlorides of the resp. nitrogen bases were the only solids isolated. The crystal structure of the amination product was determined by x-ray diffraction and shown to be N-amino-3,5-dimethylpyridinium chloride (I). The changes in N-N and C-N distances and C-N-C bond angles produced by the amination of 3,5-lutidine are discussed in terms of the changes in hybridization of the bonding orbitals of the heterocyclic nitrogen.

L10 ANSWER 32 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:452692 HCAPLUS
DOCUMENT NUMBER: 113:52692
TITLE: Regulation of aspartate aminotransferase messenger ribonucleic acid level by testosterone
AUTHOR(S): Franklin, R. B.; **Qian, K.**; Costello, L. C.
CORPORATE SOURCE: Baltimore Coll. Dent. Surg., Univ. Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Steroid Biochemistry (1990), 35(5), 569-74
CODEN: JSTBBK; ISSN: 0022-4731
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Testosterone induced a 2-3-fold increase in precursor mitochondrial aspartate aminotransferase (pmAAT) mRNA level in both rat ventral prostate and mini-pig prostate cultures. The pmAAT mRNA induction occurred 30 min after testosterone treatment and was maximal by 1.5 h. Prostatic mAAT activity was also induced by testosterone with a 1-2 h lag period. The time-course of induction of pmAAT mRNA, pmAAT activity, and mAAT activity was consistent with stimulation of mRNA synthesis followed by increase synthesis and import of pmAAT into mitochondria. The effect of testosterone on pmAAT mRNA was specific, because the increase in pmAAT was ≥2-fold greater than the increase in poly(A+) RNA. Thus, testosterone stimulated mAAT activity by induction of pmAAT mRNA. Evidently, a major physiol. effect of testosterone is increased pmAAT mRNA steady-state levels which result in increased pmAAT synthesis and increased mAAT activity. These changes ultimately result in increased citrate production by prostate epithelial cells.

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=> => d stat que nos
L3              STR
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L6            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5
L7           18 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "COGAN D A"/AU OR ("COGAN
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L8           78 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HAO M"/AU OR "HAO M H"/AU OR
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L10          32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L7 OR L9) NOT L6
L11           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND (CYTOKINE)
L12          15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND INHIBIT?
L13           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L11 OR L12) NOT (L6 OR L10)


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L13  ANSWER 1 OF 8  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2003:991342  HCAPLUS
DOCUMENT NUMBER:          140:42161
TITLE:                    Preparation of substituted 3-amino-thieno[2,3-
                          b]pyridine-2-carboxylic acid amide compounds and
                          processes for preparing and their uses as
                          inhibitors of IκB kinase complex
INVENTOR(S):              Cywin, Charles L.; Chen, Zhidong; Emeigh, Jonathan;
                          Fleck, Roman Wolfgang; Hao, Ming-hong;
                          Hickey, Eugene; Liu, Weimin; Marshall, Daniel Richard;
                          Morwick, Tina; Nemoto, Peter; Sorcek, Ronald John;
                          Sun, Sanxing; Wu, Jiang-ping
PATENT ASSIGNEE(S):       Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE:                   PCT Int. Appl., 165 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     WO 2003103661         A1    20031218    WO 2003-US17343         20030603
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2483890            AA    20031218    CA 2003-2483890         20030603
     US 2004053957         A1    20040318    US 2003-453175          20030603
     US 6964956            B2    20051115
     BR 2003011605         A     20050222    BR 2003-11605           20030603
     EP 1513516            A1    20050316    EP 2003-736796          20030603
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2005530816         T2    20051013    JP 2004-510780          20030603
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US 2004180922	A1	20040916	US 2003-730172	20031206
US 6974870	B2	20051213		
NO 2004004599	A	20050216	NO 2004-4599	20041025
US 2005288285	A1	20051229	US 2005-206707	20050818
PRIORITY APPLN. INFO.:			US 2002-386312P	P 20020606
			US 2003-457867P	P 20030326
			US 2003-453175	A1 20030603
			WO 2003-US17343	W 20030603

OTHER SOURCE(S): MARPAT 140:42161

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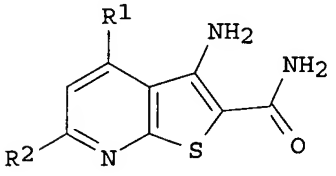

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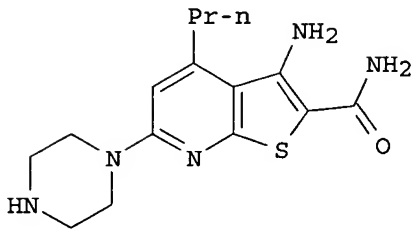

II

AB Title compds. I [R1 = (un)substituted-Ph, -heteroaryl, -heterocyclyl, -alkyl, -alkoxy, etc.; R2 = (un)substituted-alkyl, -alkoxy, -alkylamino, -alkylthio, -Ph, -heterocyclyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as **inhibitors** of the kinase activity of the IκB kinase (IKK) complex. Thus, e.g., II was prepared in five steps by cyclization of Me 2-hexynoate with 2-cyanothioacetamide in the presence of morpholine to provide intermediate mercaptopyridone which is S-alkylated with 2-bromoacetamide, converted to the O-triflate derivative, reacted with 1-BOC-piperazine and deprotected. I possessed IC50's of 10 μM or below in assays for **inhibition** of IKKβ. The compds. are therefore useful in the treatment of IKK mediated diseases including autoimmune diseases, inflammatory diseases and cancer. Also disclosed are pharmaceutical compns. comprising these compds. and processes for preparing these compds.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:432596 HCAPLUS

TITLE: Biological evaluation of BIRB 796 analogs as potent **inhibitors** of P38 MAP

AUTHOR(S): Cirillo, Pier F.; Capolino, Alison; Gilmore, Thomas; Graham, Anne; **Hao, Ming-Hong**; Hickey, Eugene; Kroe, Rachel; Moriak, Monica; Madwed, Jeff; Moss, Neil; Nelson, Richard; Pargellis, Christopher; Regan, John; Torcellini, Carol; Tsang, Michele; Swinamer, Alan

CORPORATE SOURCE: Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT, USA

SOURCE: Abstracts, 31st Northeast Regional Meeting of the American Chemical Society, Saratoga Springs, NY, United States, June 15-18 (2003), 60. American Chemical Society: Washington, D. C. CODEN: 69EBFV

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB The N-pyrazole-N'-naphthylurea BIRB 796 is a potent, selective and orally

active **inhibitor** of p38 MAP kinase and TNF-α production It is currently in Phase II clin. trials for the treatment of inflammatory diseases. The compound **inhibits** p38 by occupying an allosteric site created by the movement of the conserved DFG motif on the activation loop, as well as by occupying the ATP and kinase specificity pockets. In the ATP pocket, a key hydrogen bond is established between the oxygen atom of the morpholine and NH of Met109 on the hinge region. The structure-activity relationship for a series of BIRB 796 analogs is presented. Changes to the hydrogen-bond acceptor heterocycle, the nature and length of its linker to the naphthalene core, and the nature of the groups appended to the pyrazole moiety, were investigated.

L13 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:55370 HCAPLUS
DOCUMENT NUMBER: 140:5280
TITLE: Design and synthesis of dipeptide nitriles as reversible and potent Cathepsin S **inhibitors** . [Erratum to document cited in CA138:56234]
AUTHOR(S): Ward, Yancey D.; Thomson, David S.; Frye, Leah L.; Cywin, Charles L.; Morwick, Tina; Emmanuel, Michel J.; Zindell, Renee; McNeil, Daniel; Bekkali, Younes; Girardot, Marc; Hrapchak, Matt; DeTuri, Molly; Crane, Kathy; White, Della; Pav, Susan; Wang, Yong; **Hao, Ming-Hong**; Grygon, Christine A.; Labadia, Mark E.; Freeman, Dorothy M.; Davidson, Walter; Hopkins, Jerry L.; Brown, Maryanne L.; Spero, Denice M.
CORPORATE SOURCE: Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877-0368, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(5), 882
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The name of author Marc Girardot was incorrect in the version published on the Web 10/31/2002 (ASAP) and in the Dec. 5, 2002 issue (Volume 45, Number 25, pp 5471-5482). The correct electronic version of the manuscript was published on 01/20/2003.

L13 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:835002 HCAPLUS
DOCUMENT NUMBER: 138:56234
TITLE: Design and synthesis of dipeptide nitriles as reversible and potent cathepsin S **inhibitors**
AUTHOR(S): Ward, Yancey D.; Thomson, David S.; Frye, Leah L.; Cywin, Charles L.; Morwick, Tina; Emmanuel, Michel J.; Zindell, Renee; McNeil, Daniel; Bekkali, Younes; Giradot, Marc; Hrapchak, Matt; DeTuri, Molly; Crane, Kathy; White, Della; Pav, Susan; Wang, Yong; **Hao, Ming-Hong**; Grygon, Christine A.; Labadia, Mark E.; Freeman, Dorothy M.; Davidson, Walter; Hopkins, Jerry L.; Brown, Maryanne L.; Spero, Denice M.
CORPORATE SOURCE: Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877-0368, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(25), 5471-5482
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:56234

AB The specificity of the immune response relies on processing of foreign proteins and presentation of antigenic peptides at the cell surface. **Inhibition** of antigen presentation, and the subsequent activation of T-cells, should, in theory, modulate the immune response. The cysteine protease cathepsin S performs a fundamental step in antigen presentation and therefore represents an attractive target for **inhibition.** Herein, the authors report a series of potent and reversible Cathepsin S **inhibitors** based on dipeptide nitriles. These **inhibitors** show nanomolar **inhibition** of the target enzyme as well as cellular potency in a human B cell line. The first x-ray crystal structure of a reversible **inhibitor** cocrystd. with cathepsin S is also reported.

L13 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:617864 HCAPLUS
TITLE: Design and synthesis of novel cathepsin S **inhibitors**
AUTHOR(S): Spero, Denice M.; Ward, Yancey D.; Thomson, David; Frye, Leah; Cywin, Charles; Morwick, Tina; Emmanuel, Michel; Zindell, Renee; McNeil, Dan; Bekkali, Younes; Hrapchak, Matt; Crane, Kathy; White, Della; Wang, Yong; **Hao, Ming-Hong**; Grygon, Chris; Labadia, Mark; Brown, Maryanne
CORPORATE SOURCE: Medicinal Chemistry Department, Boehringer Ingelheim Pharmaceuticals, Inc, Ridgefield, CT, 06877, USA
SOURCE: Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), MEDI-010. American Chemical Society: Washington, D. C.
CODEN: 69CZPZ
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB The specificity of the immune response relies on processing of foreign proteins and presentation of antigenic peptides at the cell surface. **Inhibition** of antigen presentation, and the subsequent activation of T-cells, should, in theory, modulate the immune response. The cysteine protease Cathepsin S provides a key step in antigen presentation and therefore represents an attractive target for **inhibition.** Herein, we report a series of potent and reversible Cathepsin S **inhibitors.** These **inhibitors** show nanomolar **inhibition** of the target enzyme as well as cellular potency in a human B cell line. The X-ray crystal structure of a reversible **inhibitor** co-crystallized with Cathepsin S is also reported.

L13 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:380570 HCAPLUS
DOCUMENT NUMBER: 135:5453
TITLE: Preparation of aromatic heterocyclic substituted urea derivatives as non-steroidal anti-inflammatory agents
INVENTOR(S): Breitfelder, Steffen; Cirillo, Pier F.; **Hao, Ming-Hong**; Hickey, Eugene R.; Sharma, Rajiv; Sun, Sanxing; Takahashi, Hidenori
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001036403	A1	20010525	WO 2000-US31582	20001116
W: AE, AU, BG, BR, BY, CA, CN, CZ, EE, HR, HU, ID, IL, IN, JP, KR, KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, UZ, VN, YU, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2389360	AA	20010525	CA 2000-2389360	20001116
EP 1232150	A1	20020821	EP 2000-978751	20001116
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR				
US 6492393	B1	20021210	US 2000-714539	20001116
JP 2003514808	T2	20030422	JP 2001-538892	20001116
US 2003125354	A1	20030703	US 2002-271301	20021015
PRIORITY APPLN. INFO.:			US 1999-165903P	P 19991116
			US 2000-714539	A3 20001116
			WO 2000-US31582	W 20001116

OTHER SOURCE(S): MARPAT 135:5453

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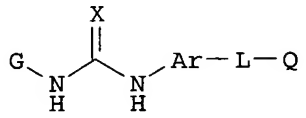

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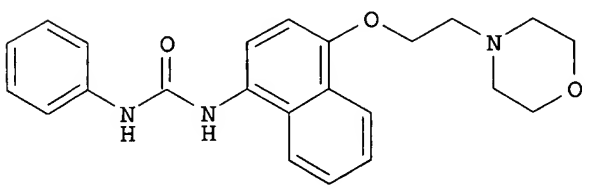

II

AB Title compds. (I) [wherein G = (un)substituted (non)aromatic carbocycle or heterocycle; Ar = (un)substituted Ph, (tetrahydro)naphthyl, (tetrahydro)quinolinyl, (tetrahydro)isoquinolinyl, (dihydro)benzofuranyl, dihydrobenzothienyl, indolenyl, benzothiophenyl, benzimidazolyl, indanyl, indenyl, or indolyl; L = (un)substituted (un)saturated C chain with one or more methylene groups optionally independently replaced by O, N, or S(O)m; Q = (un)substituted Ph, naphthyl, pyridinyl, pyrimidinyl, pyridazinyl, (benz)imidazolyl, furanyl, thenyl, pyranyl, etc.; m = 0-2; X = O or S] were prepared as **cytokine** production **inhibitors** for use as non-steroidal anti-inflammatory agents. Thus, 4-[2-(morpholin-4-yl)ethoxy]naphth-1-ylamine was treated sequentially with phosgene and 5-tert-butyl-2-methylaniline in CH2Cl2 to give II (42%). In a **cytokine** production **inhibition** assay, II **inhibited** TNFα in lipopolysaccharide stimulated THP cells with IC50 < 10 μM.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:74177 HCAPLUS

DOCUMENT NUMBER: 128:140551

TITLE: Absolute Stereochemistry of Soulattrolide and Its Analogs

AUTHOR(S): Shi, Xiongwei; Attygalle, Athula B.; Liwo, Adam; **Hao, Ming-Hong**; Meinwald, Jerrold; Dharmaratne, H. Ranjith W.; Wanigasekera, W. M. Anoja P.
CORPORATE SOURCE: Department of Chemistry, Cornell University, Ithaca, NY, 14853, USA
SOURCE: Journal of Organic Chemistry (1998), 63(4), 1233-1238
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The absolute stereochem. of a group of dipyranocoumarins, some of which are potent **inhibitors** of HIV-1 reverse transcriptase, was examined Soulattrolide and cordatolide B, two of these dipyranocoumarins, were converted to α-methoxy-α-(trifluoromethyl)phenylacetate (MTPA) derivs. and investigated by 1H NMR spectroscopy. A correlation of 1H NMR chemical shift differences with those predicted by Mosher's concept alone was inadequate to assign confidently the absolute configurations, due to the fact that in both of these mols. too few protons are present on one side of the MTPA plane. However, energetically favored conformations obtained by mol. mechanics calcns. provided satisfactory rationalizations for the observed anisotropic shifts in 1H NMR data. The combined results of the two techniques allow us to assign the absolute configuration of both soulattrolide and cordatolide B as (10S,11R,12S). The absolute configurations of the other structurally related **inhibitors**, including inophyllums B, D, and P, costatolide, calanolides A, B, and C, and cordatolide A, are also assigned on the basis of chemical conversions and correlations of their chiroptical properties.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:554415 HCAPLUS
DOCUMENT NUMBER: 119:154415
TITLE: Unfolding and refolding of the native structure of bovine pancreatic trypsin **inhibitor** studied by computer simulations
AUTHOR(S): **Hao, M. H.**; Pincus, M. R.; Rackovsky, S.; Scheraga, H. A.
CORPORATE SOURCE: Baker Lab. Chem., Cornell Univ., Ithaca, NY, 14853-1301, USA
SOURCE: Biochemistry (1993), 32(37), 9614-31
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new procedure for studying the folding and unfolding of proteins, with an application to bovine pancreatic trypsin **inhibitor** (BPTI), is reported. The unfolding and refolding of the native structure of the protein are characterized by the dimensions of the protein, expressed in terms of the three principal radii of the structure considered as an ellipsoid. A dynamic equation, describing the variations of the principal radii on the unfolding path, and a numerical procedure to solve this equation are proposed. Expanded and distorted conformations are refolded to the native structure by a dimensional-constraint energy minimization procedure. A unique and reproducible unfolding pathway for an intermediate of BPTI lacking the [30,51] disulfide bond is obtained. The resulting unfolded conformations are extended; they contain near-native local structure, but their longest principal radii are more than 2.5 times greater than that of the native structure. The most interesting finding is that the majority of expanded conformations, generated under various

conditions, can be closely refolded to the native structure, as measured by the correct overall chain fold, by the rms deviations from the native structure of only 1.9-3.1 Å, and by the energy differences of about 10 kcal/mol from the native structure. Introduction of the [30,51] disulfide bond at this stage, followed by minimization, improves the closeness of the refolded structures to the native structure, reducing the rms deviations to 0.9-2.0 Å. The unique refolding of these expanded structures over such a large conformational space implies that the folding is strongly dictated by the interactions in the amino acid sequence of BPTI. The simulations indicate that, under conditions that favor a compact structure as mimicked by the volume constraints in the authors' algorithm, the expanded conformations have a strong tendency to move toward the native structure; therefore, they probably would be favorable folding intermediates. The results presented here support a general model for protein folding, i.e., progressive formation of partially folded structural units, followed by collapse to the compact native structure. The general applicability of the procedure is also discussed.

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